Short Curriculum Vitae of Prof. Dr. Konstantin M. Neyman



Personal Details

Official address: Dept. de Ciència de Materials i Química Física, Universitat de Barcelona, c/Martí i Franquès 1, 08028 Barcelona, Spain

E-mail: konstantin.neyman_AT_icrea.cat
www.icrea.cat/community/icreas/17437/konstantin-neyman

Language skills: English, German, Spanish, Catalan, Russian

ORCID 0000-0002-5242-5567, Researcher ID F-4055-2011, Scopus ID 7004174897
Google Scholar https://scholar.google.com/citations?user=GTuSYqcAAAAJ&hl=en

Education

1973-1978	Study of chemistry, Novosibirsk State University, USSR; Diploma (MSc) in Inorganic Chemistry
1978-1980	Research trainee, Institute of Inorganic Chemistry, USSR Academy of Sciences, Krasnoyarsk
1986	PhD in Chemistry, Institute of Inorganic Chemistry, USSR Academy of Sciences, Novosibirsk

Employment History

1980-1989	Scientist, Institute of Chemistry & Chemical Technology, USSR Academy of Sciences, Krasnoyarsk
1989-1992	Senior Scientist, Head of the Quantum Chemistry Group, Institute of Chemistry of Natural Organic Materials, Russian Academy of Sciences, Krasnoyarsk
1993-1998	Research Associate, Institute of Physical and Theoretical Chemistry, TU München, Germany
1998-2002	Research Associate, Dept. of Chemistry, Ludwig-Maximilians-Universität, Munich, Germany
2002-2003	Research Associate, Dept. of Chemical Physics, Fritz-Haber Inst. of the MPG, Berlin, Germany
2003-now	ICREA* Professor, Dept. de Ciència de Materials i Quím. Física & Inst. de Quím. Teòr. i Comp., Universitat de Barcelona; *Reactivity of Nanostructures* group leader. Promoted: 2007, 2012, 2017, 2022

Other Professional Activities (selection)

1985-1991	Assistant Professor, Senior Lecturer, Chair of Inorganic Chemistry, Krasnoyarsk State University
1991-1992	Alexander von Humboldt research fellow (with Prof. N. Rösch), TU München, Germany
2003	Habilitation and Venia Legendi in Theoretical Chemistry at TU München, Germany
2009	Invited Visiting Professor, Universidad Nacional del Sur, Bahía Blanca, Argentina
2010	Accreditation in Advanced Research, Catalan University Quality Assurance Agency, Spain
2010-2014	COST Action MP0903 "Nanoalloys", Leader of the Workgroup "Catalysis"
2013	Invited Visiting Professor (1.5 months), SCBE, Nanyang Technological University, Singapore
2017	Invited Visiting Professor (5.5 months), Uppsala University, Ångström Lab., Uppsala, Sweden
2017	Chalmers Jubilee Professor (2 month), Chalmers University of Technology, Gothenburg, Sweden
2018	Visiting Professor (5.5 months), Boreskov Institute of Catalysis, Novosibirsk, Russia
2009-2026	Invited Visiting Scientist, Universität Erlangen-Nürnberg, Germany (Profs. J. Libuda, A. Görling)
2024	Guest-Professor (3.5 months), TU Wien, Vienna, Austria (Prof. G. Rupprechter)
2025	Invited Visiting Scientist, National University of Singapore, Singapore (Ass. Prof. S. Kozlov)
2026	Invited Visiting Scientist (5 weeks), Universität zu Kiel, Kiel, Germany (Prof. S. Schauermann)

Awards, Research Fellowships, Supervision of Students, etc.

Since 1982	Supervisor of Diploma/MSc studies: P.V. Avramov (1982), O.G. Senotrusov (1986); Barcelona - A. Bruix (2009), J. Toda (2011), S. Olobardi (2019), N. Danielis (2020), E. Zerbato (2022)
Since 1985	Supervisor of PhD studies: V.A. Nasluzov (1985-1989); Barcelona – A. Bruix (2009-2014, *excellent - cum laude*), S.M. Kozlov (2011-2015, *excellent - cum laude*), A. Figueroba (2013-2017, *excellent*), L. Vega (2017-2021, *excellent - cum laude*) , J. Quinlivan Domínguez (2021-2025, *excellent*), P. Castro Latorre (2020-2025, *excellent*), R. Farris (2021-2025, *excellent - cum laude*)
1991-1992	Research fellowship of the Alexander von Humboldt Foundation, Germany
1991	Senior Scientist in Physical Chemistry (awarded by the USSR Supreme Attestation Committee)
1992	Docent, Chair of Inorganic Chemistry (awarded by the USSR State Committee)
Since 2000	Advisor of PhD students: TU München - D.I. Ganyushin (2004); C. Inntam (2005); K.H. Lim (2006), A.B. Mohammad (2008); Uni. Barcelona - S. González (2007), F. Viñes (2008)
Since 2006	Academic host of: Dr. C. Loschen (A. v. Humboldt grant; 2006-2007), Dr. I. Yudanov (PIV; 2008), Prof. G.N. Vayssilov (HPC-Europa; 2009-2010), Dr. H. Aleksandrov (EXTESP 2011-12; 2013-19)
2012	A. von Humboldt grant for research at FAU Erlangen-Nürnberg (Germany, July-August 2012)
2016	Visiting Professor award, Uppsala University, Uppsala, Sweden (2017)
2016	Chalmers Jubilee Professor award, Chalmers Uni. of Technology, Gothenburg, Sweden (2017)
2022	Invited Scientist award, Collaborative Research Center CLINT, Uni. Erlangen, Germany (2023)

* ICREA - Catalan Institute for Research and Advanced Studies; since 16/11/2003

Attraction of Funds, selection since 2012

2012 Grant FP7-NMP.2012.1.1-1 ChipCAT "Design of thin-film nanocatalysts for on-chip fuel cell technology", reference 310191, EU. 12/2012-11/2016 (PI)
2012 "Theoretical modelling of the reactivity of nanostructures relevant to catalysis and to energy technologies", grant CTQ2012-34969 Spanish MINECO-FEDER 01/2013-12/2015 (PI)
2014 2 grants to organize a General Meeting of the COST Action CM1104, 11/2014, Barcelona, Spain
2014 Recognized research group grant 2014 SGR 97, PI F. Illas, Generalitat de Catalunya, Spain 2014-2016
2016 "Comprensión, control y optimización en catálisis heterogénea y fotocatálisis en la nanoescala. Aplicación a la conversión de dióxido de carbono y a la producción de hidrogeno", grant CTQ2015-64618-R Spanish MINECO/FEDER, 01/2016-09/2019 (PIs F. Illas & S.T. Bromley)
2016 Horizon-2020 grant MATERIALS NETWORKING "Enhancing the scientific capacity of the Faculty of Chemistry and Pharmacy at Sofia University as leading regional research and innovation centre in the area of advanced functional materials", EU, reference Nº 692146; 09/2016-08/2019 (PI)
2017 Salvador de Madariaga grant, PRX17/00348, Min. Educ., Cultura y Deporte, Spain, 01-06/2018 (PI)
2018 Secured pre-doctoral grant 2018FI-B-00384 for Lorena Vega, AGAUR, Spain, 2018-2021 (Supervisor)
2018 Recognized group "Computational Materials Science Lab.", 2017SGR13, GenCat, Spain 2017-2021
2018 Grant "María de Maeztu Unit of Excellence 2017" MDM-2017-0767 for the Institut de Quimica Teòrica i Comput., Uni. Barcelona, Min. de Ciencia, Innovación y Universidades, Spain 2018-2022
2019 Electronic Structure of Molecules and Solids, grant PGC2018-093863-B-C22, Spanish Min. de Ciencia, Innovación y Universidades/FEDER, 2019-2022 (Co-PI)
2019 Beatriu de Pinós grant 2018BP00190 for Dr. Albert Bruix "Development of a computational platform for kinetic studies of complex nanostructured catalysts", AGAUR, Catalonia, Spain, 2020-2023 (PI)
2020 Pre-doctoral grant PRE2019-088979 for Pablo Castro Latorre, MICIN, Spain 2021-2025 (Supervisor)
2021 Pre-doctoral grant PRE2020-091903 for Riccardo Farris, MICIN, Spain 2021-2025 (Supervisor)
2022 Computational modelling of complex materials for advanced technologies, grant PID2021-128217NB-I00, Spanish MCIUN - Min. de Ciencia, Innovación y Universidades/FEDER, 2022-2025 (Co-PI)
2022 Grant "María de Maeztu Unit of Excellence" CEX2021-001202-M for the Institut de Quimica Teòrica i Computacional, Universitat de Barcelona, Ministerio de Ciencia e Innovación, Spain 2023-2026
2022 Recognized research "Grup d'Estructura Electrònica", 2021 SGR 00286, GenCat, Spain 2022-2024
2023 Salvador de Madariaga grant, PRX22/00367, Ministerio de Universidades, Spain, 02-05/2024 (PI)
2023 Towards efficient hydrogen production with new hybrid electrocatalysts, grant 2023 CLIMA 00064, AGAUR, Catalonia, Spain, 2024-2025
2025 Computational modelling of low-dimensional materials: structure, magnetism and electron transport, grant PID2024-157317NB-I00, Spanish MCIUN/FEDER, 2025-2029

Selected Managerial Activities

Spanish representative in the Management Committee (member or substitute) of the COST Actions: CM0904 "Intermetallic compounds as catalysts" (2010-2014); MP0903 "Nanoalloys as advanced materials" (2010-2014; "Catalysis" Workgroup leader); CM1104 "Reducible oxides" (2012-2016); CA18234 "Computational materials sciences for efficient water splitting with nanocrystals from abundant elements" (2019-2021). Steering Committee Chairman - Intern. project EXTREME, Uni. Sofia, Bulgarian Ministry of Science (2021-2024).

Organization of Conferences, selection since 2018

Organizer, Int. Symposium "Density Functional Theory, Sorption and Catalysis", Garching, DE, 2023; Scientific Committee, Int. School "Catalyst Design: From Molecular to Industrial Level", Novosibirsk, RU, 2021; Co-organizer, Int. Symposium on the DFT Modelling of Materials Relevant for Water Splitting, Barcelona, ES, 2020; Organizer, Symposia on Nano-alloys, 28th - 27th Int. Materials Research Congresses, Cancún, MX, 2019 - 2018

Editorial Activities

Advisory/Editorial board member: *Adv. Phys. Chem.* 2009-17, *J. Siberian Fed. Univ.: Chem.* 2013- *J. Multiscale Model.* 2017-, *Materials* 2018-, *Sci* 2018-2024, *Nanomaterials 20*19-.

Research Focuses

Innovative first-principles computational modelling of structure and reactivity of metal, bimetallic and metal-oxide nanoparticles and based on them nano-materials for catalysis and sustainable energy technologies.

Publications and Conference Presentations (summary)

1 book, 9 book chapters, 219 articles, 166 invited talks & 235 other scientific presentations. 16000+ Google-Scholar citations, ***H-index 68***. 30+ articles in premier journals such as *ACS Nano, ACS Catal.* (3), *Angew. Chem. Int. Ed.* (5), *Appl. Catal. B* (3), *Chemistry: Eur. J.* (3), *Chem. Mater.*, *Chemical Sci.*, *Chem. Soc. Rev.*, *Chemistry of Materials*, *J. Am. Chem. Soc.* (4), *J. Catal.* (4) *J. Mater. Chem./A* (3), *Nanoscale* (2), *NPG Asia Materials*, *Nature Materials* (3)

September 15th, 2026

List of Publications and Presentations of Research Results

ICREA Professor, Dr. Konstantin M. Neyman September 15th, 2026

Publications

Articles in refereed journals

2026

219. R. Farris, E. Telari, N. Artrith, **K.M. Neyman**, A. Bruix. Bayesian neural networks versus deep ensembles for uncertainty quantification in machine learning interatomic potentials. - Mach. Learn.: Sci. Technol. 7 (2026) 055014 (1-19), doi: 10.1088/2632-2153/ae9de8.

218. J.E. Quinlivan Domínguez, M.-P. Verner Christiansen, **K.M. Neyman**, B. Hammer, A. Bruix. Efficient grand canonical global optimization with on-the-fly-trained machine-learning interatomic potentials. - J. Chem. Phys. 165 (2026) 034115 (1-13), doi: 10.1063/5.0302876.

217. P. Castro-Latorre, A. Bruix, H. Grönbeck, **K.M. Neyman**. How PtO_x/CeO_2 nanostructures catalyze CO oxidation at very low temperature. - ACS Catal. 16 (2026) 12009-12020, doi: 10.1021/acscatal.6c01003

216. Y.V. Yudanov, S.S. Laletina, **K.M. Neyman**. CO adsorption on Pd nanoparticles: Assignment of experimental C-O vibrational frequencies by DFT calculations. - J. Phys. Chem. C 130 (2026) 2562-2570, doi: 10.1021/acs.jpcc.5c08124

215. P.A. Fredersdorff, J. Smyczek, C. Schröder, P. Fröhlich, P. Kohlmorgen, S. Appelfeller, **K. Neyman**, S. Schauermann. Pd/Cu single atom alloys for selective alcohol dehydrogenation: from single crystalline to nanostructured model catalysts. - Angew. Chem. Int. Ed. 65 (2026) e21885 (1-11), doi: 10.1002/anie.202521885; Angew. Chem. 138 (2026) e21885 (1-11), doi: 10.1002/ange.202521885

214. P.A. Fredersdorff, J. Smyczek, C. Schröder, P. Kohlmorgen, P. Fröhlich, P. Hubert, S. Appelfeller, **K.M. Neyman**, S. Schauermann. Surface composition of Pd/Cu(111) single-atom alloys and its impact on selective non-oxidative butanol dehydrogenation. - Surf. Sci. 766 (2026) 122904 (1-14). doi: 10.1016/j.susc.2025.122904

2025

213. B.S. Karapenchev, I.Z. Koleva, **K.M. Neyman**, H.A. Aleksandrov. DFT study of the stability and reducibility of Hf-doped ceria nanoparticles. - J. Phys. Chem. C 129 (2025) 7704-7716. doi: 10.1021/acs.jpcc.4c08636

212. X. Xie, V. Briega-Martos, P. Alemany, A. Lekshmi Mohandas Sandhya, T. Skála, M. Gamón Rodríguez, M. Dopita, M. Vorochta, A. Bruix, S. Cherevko, **K.M. Neyman**, I. Matolínová, I. Khalakhan. Balancing activity and stability through compositional engineering of ternary PtNi-Au alloy ORR catalysts. - ACS Catal. 15 (2025) 234-245. doi: 10.1021/acscatal.4c05269

2024

211. R. Farris, **K.M. Neyman**, A. Bruix. Determining the chemical ordering in nanoalloys by considering atomic coordination types. - J. Chem. Phys. 161 (2024) 134114. doi: 10.1063/5.0214377

210. **K.M. Neyman**, P. Alemany. Chemical orderings in CuCo nanoparticles: Topological modeling using DFT calculations. - Nanomaterials 14 (2024) 1242. doi: 10.3390/nano14151242

209. L. Piliai, P. Castro-Latorre, F. Pchálek, S. Oveysipoor, Y. Kosto, I. Khalakhan, T. Skála, **K.M. Neyman**, P. Alemany, M. Vorochta, A. Bruix, P. Matvija, I. Matolínová. Electronic and structural properties of thin iron oxide films on CeO_2. - ACS Appl. Mater. Interfaces 16 (2024) 46858-46871. doi: 10.1021/acsami.4c05542

208. R. Farris, B.V. Merinov, A. Bruix, **K.M. Neyman**. Effects of Zr dopants on properties of PtNi nanoparticles for ORR catalysis: a DFT modeling. - J. Chem. Phys. 160 (2024) 124706 (1-9). doi: 10.1063/5.0193848

2023

207. E. Zerbato, R. Farris, G. Fronzoni, **K.M. Neyman**, M. Stener, A. Bruix. Effects of oxygen adsorption on optical properties of Ag nanoparticles. - J. Phys. Chem. A 127 (2023) 10412-10424. doi: 10.1021/acs.jpca.3c05801

206. P. Castro-Latorre, **K.M. Neyman**, A. Bruix. Systematic characterization of electronic metal support interactions in ceria-supported Pt clusters. - J. Phys. Chem. C 127 (2023) 17700-17710. doi: 10.1021/acs.jpcc.3c03383

205. E.M. Slavinskaya, A.I. Stadnichenko, J.E. Quinlivan Domínguez, O.A. Stonkus, M. Vorokhta, B. Šmíd, P. Castro-Latorre, A. Bruix, **K.M. Neyman**, A.I. Boronin. States of Pt/CeO_2 catalysts for CO oxidation below room temperature. - J. Catal. 421 (2023) 285-299. doi: 10.1016/j.jcat.2023.03.004

204. X. Xie, V. Briega-Martos, R. Farris, M. Dopita, M. Vorokhta, T. Skála, I. Matolínová, **K.M. Neyman**, S. Cherevko, I. Khalakhan. Optimal Pt-Au alloying for efficient and stable oxygen reduction reaction catalyst. - ACS Appl. Mater. Interfaces 15 (2023) 1192-1200. doi: 10.1021/acsami.2c18655

2022

203. J.E. Quinlivan Domínguez, **K.M. Neyman**, A. Bruix. Stability of oxidized states of free-standing and ceria-supported PtO_x particles. - J. Chem. Phys. 157 (2022) 094709 (1-11). doi: 10.1063/5.0099927

202. O. Bezkrovnyi, A. Bruix, D. Blaumeiser, L. Piliai, S. Schötz, T. Bauer, I. Khalakhan, T. Skála, P. Matvija, P. Kraszkiewicz, M. Pawlyta, M. Vorokhta, I. Matolínová, J. Libuda, **K.M. Neyman**, L. Kępiński. Metal-support interaction and charge distribution in ceria-supported Au particles exposed to CO. - Chem. Mater. 34 (2022) 7916-7936. doi: 10.1021/acs.chemmater.2c01659

201. **K.M. Neyman**, S.M. Kozlov. Quantifying interactions on interfaces between metal particles and oxide supports in catalytic nanomaterials. - NPG Asia Materials 14 (2022) 59 (1-8). doi: 10.1038/s41427-022-00405-4

200. L. Vega, J. Garcia-Cardona, F. Viñes, P.L. Cabot, **K.M. Neyman**. Nanostructuring determines poisoning: Tailoring CO adsorption on PtCu bimetallic nanoparticles. - Mater. Adv. 3 (2022) 4159-4169. doi: 10.1039/D2MA00196A + front cover doi: 10.1039/d2ma90053j

199. L. Vega, F. Viñes, **K.M. Neyman**. Unravelling morphological and topological energy contributions of metal nanoparticles. - Nanomaterials 12 (2022) 17. doi: 10.3390/nano12010017

2021

198. V.A. Nasluzov, E.A. Ivanova-Shor, A.M. Shor, S.S. Laletina, **K.M. Neyman**. Adsorption and oxidation of CO on ceria nanoparticles exposing single-atom Pd and Ag: A DFT modelling. - Materials 14 (2021) 6888. doi: 10.3390/ma14226888. ***Feature paper.***

197. L. Vega, H.A. Aleksandrov, R. Farris, A. Bruix, F. Viñes, **K.M. Neyman**. Chemical ordering in Pt-Au, Pt-Ag and Pt-Cu nanoparticles from density functional calculations using a topological approach. - Mater. Adv. 2 (2021) 6589-6602. doi: 10.1039/D1MA00529D + front cover doi: 10.1039/D1MA90103F

196. N. Danielis, L. Vega, G. Fronzoni, M. Stener, A. Bruix, **K.M. Neyman**. AgPd, AuPd, and AuPt nanoalloys with Ag- or Au-rich compositions: Modeling chemical ordering and optical properties. - J. Phys. Chem. C 125 (2021) 17372-17384. doi: 10.1021/acs.jpcc.1c04222

195. A.I. Boronin, E.M. Slavinskaya, A. Figueroba, A.I. Stadnichenko, T.Yu. Kardash, O.A. Stonkus, E.A. Fedorova, V.V. Muravev, V.A. Svetlichnyi, A. Bruix, **K.M. Neyman**. CO oxidation activity of Pt/CeO_2 catalysts below 0ºC: Platinum loading effects. - Appl. Catal. B: Environ. 286 (2021) 119931. doi: 10.1016/j.apcatb.2021.119931

194. M. Mamatkulov, I.V. Yudanov, A.V. Bukhtiyarov, **K.M. Neyman**. Pd single-atom sites on the surface of PdAu nanoparticles: A DFT-based Topological search for suitable compositions. - Nanomaterials 11 (2021) 122. doi: 10.3390/nano11010122. ***Editor's choice***.

2020

193. I.Z. Koleva, H.A. Aleksandrov, **K.M. Neyman**, G.N. Vayssilov. Preferential location of zirconium dopants in cerium dioxide nanoparticles and effects of doping on their reducibility: A DFT study. - Phys. Chem. Chem. Phys. 22 (2020) 26568-26582. doi: 10.1039/d0cp05456a

192. R. Brown, M. Vorokhta, I. Khalakhan, M. Dopita, T. Vonderach, T. Skála, N. Lindahl, I. Matolinová, H. Grönbeck, **K.M. Neyman**, V. Matolin, B. Wickman. Unravelling the surface chemistry and structure in highly active sputtered Pt_3Y catalyst films for the oxygen reduction reaction. - ACS Appl. Mater. Interfaces 12 (2020) 4454-4463. doi: 10.1021/acsami.9b17817

191. I. Khalakhan, L. Vega, M. Vorokhta, T. Skála, F. Viñes, Y.V. Yakovlev, **K.M. Neyman**, I. Matolínová. Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. - Appl. Catal. B: Environ. 264 (2020) 118476 (1-9). doi: 10.1016/j.apcatb.2019.118476

2019

190. S. Olobardi, L. Vega, A. Fortunelli, M. Stener, F. Viñes, **K.M. Neyman**. Optical properties and chemical ordering of Ag-Pt nanoalloys: a computational study. - J. Phys. Chem. C 123 (2019) 25482-25491. doi: 10.1021/acs.jpcc.9b07382

189. S. Liu, Z.-J. Zhao, C. Yang, S. Zha, **K.M. Neyman**, F. Studt, J. Gong. Adsorption preference determines segregation direction: A shortcut to more realistic surface models of alloy catalysts. - ACS Catal. 9 (2019) 5011-5018. doi: 10.1021/acscatal.9b00499

188. L. Vega, H.A. Aleksandrov, **K.M. Neyman**. Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications. - Chin. J. Catal. 40 (2019) 1749-1757. doi: 10.1016/S1872-2067(19)63362-0

187. T.Yu. Kardash, E.A. Derevyannikova, E.M. Slavinskaya, A.I. Stadnichenko, V.A. Maltsev, A.V. Zaikovskii, S.A. Novopashin, A.I. Boronin, **K.M. Neyman**. Pt/CeO_2 and $Pt/CeSnO_x$ catalysts for low-temperature CO oxidation prepared by plasma-arc technique. - Front. Chem. 7 (2019) 114 (1-17). doi: 10.3389/fchem.2019.00114

186. M. Mamatkulov, I.V. Yudanov, A.V. Bukhtiyarov, I.P. Prosvirin, V.I. Bukhtiyarov, **K.M. Neyman**. Pd segregation on the surface of bimetallic PdAu nanoparticles induced by low coverage of adsorbed CO. - J. Phys. Chem. C 123 (2019) 8037-8046. doi: 10.1021/acs.jpcc.8b07402

185. V.A. Nasluzov, E.A. Ivanova-Shor, A.M. Shor, **K.M. Neyman**. Silver atom, trimer and tetramer species supported on a ceria nanoparticle: A density functional study. - Surf. Sci. 681 (2019) 38-46. doi: 10.1016/j.susc.2018.11.002

184. A.I. Stadnichenko, V.V. Muravev, S.V. Koscheev, V.I. Zaikovskii, H.A. Aleksandrov, **K.M. Neyman**, A.I. Boronin. Study of active surface centers of Pt/CeO_2 catalysts prepared using

radio-frequency plasma sputtering technique. - Surf. Sci. 679 (2019) 273-283. doi: 10.1016/j.susc.2018.10.002

2018

183. H.A. Aleksandrov, I.Z. Koleva, **K.M. Neyman**, T. Tabakova, G.N. Vayssilov. Structure and reducibility of doped by yttrium cerium dioxide nanoparticles and (111) surface. - RSC Adv. 8 (2018) 33728-33741. doi: 10.1039/c8ra07014h

182. Y. Suchorski, S.M. Kozlov, I. Bespalov, M. Datler, D. Vogel, Z. Budinska, **K.M. Neyman**, G. Rupprechter. The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation. - Nature Mater. 17 (2018) 519-522. doi: 10.1038/s41563-018-0080-y Highlights https://www.altmetric.com/details/41379075/news

2017

181. O. Brummel, F. Waidhas, I. Khalakhan, M. Vorokhta, G. Kovács, H.A. Aleksandrov, **K.M. Neyman**, V. Matolín, J. Libuda. Structural transformations and adsorption properties of PtNi nanoalloy thin film electrocatalysts prepared by magnetron co-sputtering. - Electrochim. Acta 251 (2017) 427-441. doi: 10.1016/j.electacta.2017.08.062

180. A. Figueroba, A. Bruix, G. Kovács, **K.M. Neyman**. Metal-doped ceria nanoparticles: Stability and redox processes. - Phys. Chem. Chem. Phys. 19 (2017) 21729-21738. doi: 10.1039/c7cp02820b

179. H.A. Aleksandrov, S.M. Kozlov, G.N. Vayssilov, **K.M. Neyman**. Approaching complexity of alkyl hydrogenation on Pd by density functional modelling. - Phys. Chem. Chem. Phys. 19 (2017) 21514-21521. doi: 10.1039/c7cp03516k

178. Y. Lykhach, A. Bruix, S. Fabris, V. Potin, I. Matolínová, V. Matolín, J. Libuda, **K.M. Neyman**. Oxide-based nanomaterials for fuel cell catalysis: The interplay between supported Pt atoms and particles. - Catal. Sci. Technol. 7 (2017) 4315-4345 + front cover. doi: 10.1039/c7cy00710h

177. Y. Lykhach, A. Figueroba, T. Skála, T. Duchoň, N. Tsud, M. Aulická, A. Neitzel, K. Veltruská, K.C. Prince, V. Matolín, **K.M. Neyman**, J. Libuda. Redox-mediated conversion of atomically dispersed platinum to sub-nanometer particles. - J. Mater. Chem. A 5 (2017) 9250-9261. doi: 10.1039/c7ta02204b

176. G. Kovács, S.M. Kozlov, **K.M. Neyman**. Versatile optimization of chemical ordering in bimetallic nanoparticles. - J. Phys. Chem. C 121 (2017) 10803-10808. doi: 10.1021/acs.jpcc.6b11923

175. A. Neitzel, G. Kovács, Y. Lykhach, S.M. Kozlov, N. Tsud, T. Skála, M. Vorokhta, V. Matolín, **K.M. Neyman**, J. Libuda. Atomic ordering and Sn segregation in Pt-Sn nanoalloys supportted on CeO_2 thin films. - Top. Catal. 60 (2017) 522-532. doi: 10.1007/s11244-016-0709-5

174. A. Wolfbeisser, G. Kovács, S.M. Kozlov, K. Föttinger, J. Bernardi, B. Klötzer, **K.M. Neyman**, G. Rupprechter. Surface composition changes of CuNi-ZrO_2 catalysts during methane decomposition: An operando NAP-XPS and density functional study. - Catal. Today 283 (2017) 134-143. doi: 10.1016/j.cattod.2016.04.022

2016

173. V.A. Nasluzov, **K.M. Neyman**, A.M. Shor, S.S. Laletina, E.A. Ivanova-Shor. Density functional calculation of dioxygen adsorption at complexes of ceria nanoparticle with atoms, trimers and tetramers of silver. - J. Siber. Feder. Univ.: Chem. 9 (2016) 281-295 [in Russian]. doi: 10.17516/1998-2836-2016-9-3-281-295

172. S.M. Kozlov, **K.M. Neyman**. Effects of electron transfer in model catalyst composed of Pt nanoparticles on CeO_2(111) surface. - J. Catal. 344 (2016) 507-514. doi: 10.1016/j.jcat.2016.10.014

171. A. Neitzel, G. Kovács, Y. Lykhach, N. Tsud, S.M. Kozlov, T. Skála, M. Vorokhta, V. Matolín, **K.M. Neyman**, J. Libuda. Steering the formation of supported Pt–Sn nanoalloys by reactive metal-oxide interaction. - RSC Adv. 6 (2016) 85688-85697. doi: 10.1039/C6RA18801J

170. O. Brummel, F. Waidhas, F. Faisal, R. Fiala, M. Vorokhta, I. Khalakhan, M. Dubau, A. Figueroba, G. Kovács, H.A. Aleksandrov, G.N. Vayssilov, S.M. Kozlov, **K.M. Neyman**, V. Matolín, J. Libuda. Stabilization of small platinum nanoparticles on Pt-CeO_2 thin film electrocatalysts during methanol oxidation. - J. Phys. Chem. C 120 (2016) 19723-19736. doi: 10.1021/acs.jpcc.6b05962

169. A. Bruix, **K.M. Neyman**. Modeling ceria-based nanomaterials for catalysis and related applications. - Catal. Lett. 146 (2016) 2053-2080. doi: 10.1007/s10562-016-1799-1

168. H.A. Aleksandrov, **K.M. Neyman**, K.I. Hadjiivanov, G.N. Vayssilov. Can the state of platinum species be unambiguously determined by the stretching frequency of adsorbed CO probe molecule? - Phys. Chem. Chem. Phys. 18 (2016) 22108-22121. doi: 10.1039/C6CP03988J

167. A. Neitzel, A. Figueroba, Y. Lykhach, T. Skála, M. Vorokhta, N. Tsud, S. Mehl, K. Ševčíková, K.C. Prince, **K.M. Neyman**, V. Matolín, J. Libuda. Atomically dispersed Pd, Ni and Pt species in ceria-based catalysts: Principal differences in stability and reactivity. - J. Phys. Chem. C 120 (2016) 9852-9862. doi: 10.1021/acs.jpcc.6b02264

166. A. Figueroba, G. Kovács, A. Bruix, **K.M. Neyman**. Towards stable single-atom catalysts: Strong binding of atomically dispersed transition metals on the surface of nanostructured ceria. - Catal. Sci. Technol. 6 (2016) 6806-6813, highlighted in Chemical & Engineering News 94 (2016) 26-29.[1] C&EN is a weekly ACS magazine of the chemical and engineering world, providing breaking news. doi: 10.1039/c6cy00294c

165. Y. Lykhach, A. Figueroba, M. Farnesi Camellone, A. Neitzel, T. Skála, F.R. Negreiros, M. Vorokhta, N. Tsud, K.C. Prince, S. Fabris, **K.M. Neyman**, V. Matolín, J. Libuda. Reactivity of atomically dispersed Pt^{2+} species towards H_2: Model Pt-CeO_2 fuel cell catalyst. - Phys. Chem. Chem. Phys. 18 (2016) 7672-7679. doi: 10.1039/c6cp00627b

164. R. Fiala, A. Figueroba, A. Bruix, M. Václavů, A. Rednyk, I. Khalakhan, M. Vorokhta, J. Lavková, F. Illas, V. Potin, I. Matolínová, **K.M. Neyman**, V. Matolín. High efficiency Pt^{2+}-CeO_x novel thin film catalyst as anode for proton exchange membrane fuel cells. - Appl. Catal. B: Environ. 197 (2016) 262-270. doi: 10.1016/j.apcatb.2016.02.036

163. S.M. Kozlov, **K.M. Neyman**. Insights from methane decomposition on nanostructured palladium. - J. Catal. 337 (2016) 111-121. doi: 10.1016/j.jcat.2016.02.010

162. M. Vorokhta, I. Khalakhan, M. Václavů, G. Kovács, S.M. Kozlov, P. Kúš, T. Skála, N. Tsud, J. Lavková, V. Potin, I. Matolínová, **K.M. Neyman**, V. Matolín. Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. - Appl. Surf. Sci. 365 (2016) 245-251. doi: 10.1016/j.apsusc.2016.01.004

161. Y. Lykhach, S.M. Kozlov, T. Skála, A. Tovt, V. Stetsovych, N. Tsud, F. Dvořák, V. Johánek, A. Neitzel, J. Mysliveček, S. Fabris, V. Matolín, **K.M. Neyman**, J. Libuda. Counting electrons on supported nanoparticles. - Nature Mater. 15 (2016) 284-288. doi: 10.1038/nmat4500; highly cited paper.[2] Highlights https://www.altmetric.com/details/4875286/news

[1] M. Jacoby. Taking catalysis to the atomic limit. Chemists advance single-atom supported catalysts from farfetched idea to reality. http://cen.acs.org/articles/94/i39/Taking-catalysis-atomic-limit.html

[2] Cited 357 times, according to on-line Web of Science index accessed 8/4/2023

2015

160. G. Kovács, S.M. Kozlov, I. Matolínová, M. Vorokhta, V. Matolín, **K.M. Neyman**. Revealing chemical ordering in Pt-Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. - Phys. Chem. Chem. Phys. 17 (2015) 28298-28310. doi: 10.1039/c5cp01070e

159. H.A. Aleksandrov, **K.M. Neyman**, G.N. Vayssilov. Structure and stability of reduced and oxidized mononuclear platinum species on nanostructured ceria from density functional modeling. - Phys. Chem. Chem. Phys. 17 (2015) 14551-14560. doi: 10.1039/C5CP01685A

158. S.M. Kozlov, G. Kovács, R. Ferrando, **K.M. Neyman**. How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. - Chem. Sci. 6 (2015) 3868-3880. doi: 10.1039/c4sc03321c

157. P.C. Jennings, H.A. Aleksandrov, **K.M. Neyman**, R.L. Johnston. O_2 dissociation on M@Pt core-shell particles for 3d, 4d and 5d transition metals. - J. Phys. Chem. C 119 (2015) 11031-11041. doi: 10.1021/jp511598e

156. S.M. Kozlov, H.A. Aleksandrov, **K.M. Neyman**. Energetic stability of absorbed H in Pd and Pt nanoparticles in a more realistic environment. - J. Phys. Chem. C 119 (2015) 5180-5186. doi: 10.1021/jp513022m

155. S.M. Kozlov, I. Demiroglu, **K.M. Neyman**, S.T. Bromley. Reduced ceria nanofilms from structure prediction. - Nanoscale 7 (2015) 4361-4366. doi: 10.1039/C4NR07458K

2014

154. H.A. Aleksandrov, S.M. Kozlov, S. Schauermann, G.N. Vayssilov, **K.M. Neyman**. How absorbed hydrogen affects catalytic activity of transition metals. - Angew. Chem. Int. Ed. 53 (2014) 13371-13375. doi: 10.1002/anie.201405738; Angew. Chem. 126 (2014) 13589-13593. doi: 10.1002/ange.201405738

153. M.A. Sk, S.M. Kozlov, K.H. Lim, A. Migani, **K.M. Neyman**. Oxygen vacancies in self-assemblies of ceria nanoparticles. - J. Mater. Chem. A 2 (2014) 18329-18338 (+ journal cover). doi: 10.1039/c4ta02200a

152. P.C. Jennings, H.A. Aleksandrov, **K.M. Neyman**, R.L. Johnston. DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle. - Phys. Chem. Chem. Phys. 16 (2014) 26539-26545. doi: 10.1039/C4CP02147A

151. S.M. Kozlov, H.A. Aleksandrov, **K.M. Neyman**. Adsorbed and subsurface absorbed hydrogen atoms on bare and MgO(100)-supported Pd and Pt nanoparticles. - J. Phys. Chem. C 118 (2014) 15242-15250. doi: 10.1021/jp502575a

150. A. Bruix, Y. Lykhach, I. Matolínová, A. Neitzel, T. Skála, N. Tsud, M. Vorokhta, V. Stetsovych, K. Ševčíková, J. Mysliveček, R. Fiala, M. Václavů, K.C. Prince, S. Bruyère, V. Potin, F. Illas, V. Matolín, J. Libuda, **K.M. Neyman**. Maximum noble metal efficiency in catalytic materials: Atomically dispersed surface platinum. - Angew. Chem. Int. Ed. 53 (2014) 10525-10530. doi: 10.1002/anie.201402342; Angew. Chem. 126 (2014) 10693-10698. doi: 10.1002/-ange.201402342 (+ journal cover); highly cited paper in WoS.[3]

149. S.M. Kozlov, **K.M. Neyman**. O vacancies on steps on CeO_2(111) surface. - Phys. Chem. Chem. Phys. 16 (2014) 7823-7829. doi: 10.1039/C4CP00136B

148. P.C. Jennings, H.A. Aleksandrov, B.G. Pollet, **K.M. Neyman**, R.L. Johnston. A DFT study of oxygen dissociation on platinum based nanoparticles. - Nanoscale 6 (2014) 1153-1165. doi: 10.1039/C3NR04750D

2013

[3] Cited 338 times, according to on-line Web of Science index accessed on 8/4/2023

147. S.M. Kozlov, H.A. Aleksandrov, J. Goniakowski, **K.M. Neyman**. Effect of MgO(100) support on structure and properties of Pd and Pt nanoparticles with 49-155 atoms. - J. Chem. Phys. 139 (2013) 084701, 1-10 (+ journal front cover). doi: 10.1063/1.4817948

146. S.M. Kozlov, **K.M. Neyman**. Catalysis from first principles: Towards accounting for the effects of nanostructuring. -Top. Catal. 56 (2013) 867-873. doi:10.1007/s11244-013-0050-1

145. H.A. Aleksandrov, F. Viñes, W. Ludwig, S. Schauermann, **K.M. Neyman**. Tuning surface chemistry of Pd by atomic C and H: A microscopic picture. - Chem. - Eur. J. 19 (2013) 1335-1345. doi: 10.1002/chem.201201106

2012

144. C. Weilach, S.M. Kozlov, H. Holzapfel, K. Föttinger, **K.M. Neyman**, G. Rupprechter. Geometric arrangement of components in bimetallic PdZn/Pd(111) surfaces modified by CO adsorption: A combined study by density functional theory calculations, polarization-modulated infrared reflection absorption spectroscopy, and temperature-programmed desorption. - J. Phys. Chem. C 116 (2012) 18768-18778. doi: 10.1021/jp304556s

143. S.M. Kozlov, F. Viñes, N. Nilius, S. Shaikhutdinov, **K.M. Neyman**. Absolute surface step energies: Accurate theoretical methods applied to ceria nanoislands. - J. Phys. Chem. Lett. 3 (2012) 1956-1961. doi: 10.1021/jz3006942

142. Y. Lykhach, V. Johánek, H.A. Aleksandrov, S.M. Kozlov, M. Happel, T. Skála, P.S. Petkov, N. Tsud, G.N. Vayssilov, K.C. Prince, **K.M. Neyman**, V. Matolín, J. Libuda. Water chemistry on model ceria and Pt/ceria catalysts. - J. Phys. Chem. C 116 (2012) 12103-12113. doi: 10.1021/jp302229x

141. A. Migani, **K.M. Neyman**, S.T. Bromley. Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles. - Chem. Commun. 48 (2012) 4199-4201. doi: 10.1039/c2cc18046d

140. N. Nilius, S.M. Kozlov, J.-F. Jerratsch, M. Baron, X. Shao, F. Viñes, S. Shaikhutdinov, **K.M. Neyman**, H.-J. Freund. Formation of one-dimensional electronic states along the step edges of CeO_2(111). - ACS Nano 6 (2012) 1126-1133. doi: 10.1021/nn2036472

139. L.V. Moskaleva, V. Zielasek, T. Klüner, **K.M. Neyman**, M. Bäumer. CO oxidation by co-adsorbed atomic O on the Au(321) surface with Ag impurities: A mechanistic study from first-principles calculations. - Chem. Phys. Lett. 525-526 (2012) 87-91. doi: 10.1016/j.cplett.2011.12.050

2011

138. A. Bruix, F. Nazari, **K.M. Neyman**, F. Illas. On the adsorption and formation of Pt dimers on CeO_2(111) surface. - J. Chem. Phys. 135 (2011) 244708, 1-6. doi: 10.1063/1.3672102

137. C. Loschen, J. Carrasco, **K.M. Neyman**, F. Illas. Erratum: First-principles LDA+U and GGA+U study of cerium oxides: Dependence on the effective U parameter [Phys. Rev. B 75, 035115 (2007)]. - Phys. Rev. B 84 (2011) 199906(E).

136. G.N. Vayssilov, M. Mihaylov, P.St. Petkov, K.I. Hadjiivanov, **K.M. Neyman**. Reassignment of the vibrational spectra of carbonates, formates and related species on ceria: A combined density functional and infrared spectroscopy investigation. - J. Phys. Chem. C 115 (2011) 23435-23454. doi: 10.1021/jp208050a

135. G.N. Vayssilov, A. Migani, **K. Neyman**. Density functional modeling of the interactions of platinum clusters with CeO_2 nanoparticles of different size. - J. Phys. Chem. C 115 (2011) 16081-16086. doi: 10.1021/jp204222k

134. A. Bruix, A. Migani, G.N. Vayssilov, **K.M. Neyman**, J. Libuda, F. Illas. Effects of deposited Pt particles on the reducibility of CeO_2(111). - Phys. Chem. Chem. Phys. 13 (2011) 11384-11392. doi: 10.1039/c1cp20950g

133. S.M. Kozlov, G.F. Cabeza, **K.M. Neyman**. Bonding and vibrations of CH_x and CH_xO (x = 1-3) species on a Pd_{79} nanoparticle representing model catalysts. - Chem. Phys. Lett. 506 (2011) 92-97. doi: 10.1016/j.cplett.2011.02.061

132. G. Preda, A. Migani, **K.M. Neyman**, S.T. Bromley, F. Illas, G. Pacchioni. Formation of superoxide anions on ceria nanoparticles by interaction of molecular oxygen with Ce^{3+} sites. - J. Phys. Chem. C 115 (2011) 5817-5822. doi: 10.1021/jp111147y

131. G.N. Vayssilov, Y. Lykhach, A. Migani, T. Staudt, G.P. Petrova, N. Tsud, T. Skála, A. Bruix, F. Illas, K.C. Prince, V. Matolín, **K.M. Neyman**, J. Libuda. Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. - Nature Mater. 10 (2011) 310-315; highly cited paper.[4] doi: 10.1038/nmat2976

130. L.V. Moskaleva, S. Röhe, A. Wittstock, V. Zielasek, T. Klüner, **K.M. Neyman**, M. Bäumer. Silver residues as a possible key to remarkable oxidative catalytic activity of nanoporous gold. - Phys. Chem. Chem. Phys. 13 (2011) 4529-4539. doi: 10.1039/c0cp02372h

2010

129. A. Migani, G.N. Vayssilov, S.T. Bromley, F. Illas, **K.M. Neyman**. Dramatic reduction of the oxygen vacancy formation energy in ceria particles: A possible key to their remarkable reactivity at the nanoscale. - J. Mater. Chem. 20 (2010) 10535-10546. doi: 10.1039/C0JM01908A

128. A. Bruix, **K.M. Neyman**, F. Illas. Adsorption, oxidation state and diffusion of Pt atoms on the CeO_2(111) surface. - J. Phys. Chem. C 114 (2010) 14202-14207. doi: 10/1021/jp104490k

127. A. Migani, G.N. Vayssilov, S.T. Bromley, F. Illas, **K.M. Neyman**. Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. - Chem. Commun. 46 (2010) 5936-5938. doi: 10.1039/C0CC01091J

126. F. Viñes, Y. Lykhach, T. Staudt, M.P.A. Lorenz, C. Papp, H.-P. Steinrück, J. Libuda, **K.M. Neyman**, A. Görling. Methane activation by platinum: Critical role of edge and corner sites of metal nanoparticles. - Chem. - Eur. J. 16 (2010) 6530-6539. doi: 10.1002/chem.201000296

125. I.V. Yudanov, **K.M. Neyman**. Stabilization of Au at edges of bimetallic PdAu nanocrystallites. - Phys. Chem. Chem. Phys. 12 (2010) 5094-5100. doi: 10.1039/B927048E

124. **K.M. Neyman**, S. Schauermann. Hydrogen diffusion into Pd nanoparticles: Pivotal promotion by carbon. - Angew. Chem. Int. Ed. 49 (2010) 4743-4746. doi: 10.1002/anie.200904688; Diffusion von Wasserstoff in Palladium-Nanopartikeln: entscheidende Begünstigung durch Kohlenstoff. - Angew. Chem. 122 (2010) 4851-4854. doi: 10.1002/ange.200904688

2009

123. M.M. Branda, N.J. Castellani, R. Grau-Crespo, N. H. de Leeuw, N. Cruz-Hernandez, J.F. Sanz, **K.M. Neyman**, F. Illas. On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO_2(111). - J. Chem. Phys. 131 (2009) 094702, 1-11. doi: 10.1063/1.3216102

122. F. Viñes, **K.M. Neyman**, A. Görling. Carbon on platinum substrates: From carbidic to graphitic phases on the (111) surface and on nanoparticles. - J. Phys. Chem. A 113 (2009) 11963-11973. doi: 10/1021/jp903653z

121. A. Migani, **K.M. Neyman**, F. Illas, S.T. Bromley. Exploring Ce^{3+}/Ce^{4+} cation ordering in reduced ceria nanoparticles using interionic-potential and density-functional calculations. - J. Chem. Phys. 131 (2009) 064701, 1-7. doi:10.1063/1.3195063

[4] On-line Science Citation Index, Web of Science (WoS), 657 citations, accessed on 8/4/2023.

120. K.H. Lim, A.B. Mohammad, I.V. Yudanov, **K.M. Neyman**, M. Bron, P. Claus, N. Rösch. Mechanism of selective hydrogenation of α,β-unsaturated aldehydes on silver catalysts: A density functional study. - J. Phys. Chem. C 113 (2009) 13231-13240. doi: 10/1021/jp902078c

119. S.T. Bromley, I. de P.R. Moreira, **K.M. Neyman**, F. Illas. Approaching nanoscale oxides: Models and theoretical methods. - Chem. Soc. Rev. 38 (2009) 2657-2670. doi: 10.1039/b806400h

118. F. Viñes, C. Loschen, F. Illas, **K.M. Neyman**. Edge sites as a gate for subsurface carbon in palladium nanoparticles. - J. Catal. 266 (2009) 59-63. doi: 10.1016/j.jcat.2009.05.010

117. N.J. Castellani, M.M. Branda, **K.M. Neyman**, F. Illas. Density functional theory study of the adsorption of Au atom on cerium oxide: Effect of low-coordinated surface sites. - J. Phys. Chem. C 113 (2009) 4948-4954. doi: 10/1021/jp8094352

2008

116. A. Migani, C. Loschen, F. Illas, **K.M. Neyman**. Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT+U approach. - Chem. Phys. Lett. 465 (2008) 106-109. doi: 10.1016/j.cplett.2008.09.060

115. M.M. Branda, C. Loschen, **K.M. Neyman**, F. Illas. Atomic and electronic structure of cerium oxide stepped model surfaces. - J. Phys. Chem. C 112 (2008) 17643-17651. doi: 10.1021/jp806066g

114. F. Viñes, A. Desikusumastuti, T. Staudt, A. Görling, J. Libuda, **K.M. Neyman**. A combined density-functional and IRAS study on the interaction of NO with Pd nanoparticles: Identifying new adsorption sites with novel properties. - J. Phys. Chem. C 112 (2008) 16539-16549. doi: 10.1021/jp804315c

113. C. Loschen, A. Migani, S.T. Bromley, F. Illas, **K.M. Neyman**. Density functional studies of model cerium oxide nanoparticles. - Phys. Chem. Chem. Phys. 10 (2008) 5730-5738. doi: 10.1039/b805904g

112. F. Viñes, F. Illas, **K.M. Neyman**. Density functional calculations of Pd nanoparticles using a plane-wave method. - J. Phys. Chem. A 112 (2008) 8911-8915 (+ journal front cover). doi: 10.1021/jp8014854

111. A. Roldán, F. Viñes, F. Illas, J.M. Ricart, **K.M. Neyman**. Density functional studies of coinage metal nanoparticles: Scalability of their properties to bulk. - Theor. Chem. Accounts 120 (2008) 565-573. doi:10.1007/s00214-008-0423-x

110. I.V. Yudanov, A.V. Matveev, **K.M. Neyman**, N. Rösch. How the C-O bond breaks during methanol decomposition on nanocrystallites of palladium catalysts. - J. Am. Chem. Soc. 130 (2008) 9342-9352. Selected for the *JACS Select #3* "Molecular modeling of complex chemical systems".[5] doi: 10.1021/ja078322r

109. A.B. Mohammad, I.V. Yudanov, K.H. Lim, **K.M. Neyman**, N. Rösch. Hydrogen activation on silver: A computational study on surface and subsurface oxygen species. - J. Phys. Chem. C 112 (2008) 1628-1635. doi: 10.1021/jp0765190

2007

108. F. Viñes, F. Illas, **K.M. Neyman**. On the mechanism of formation of metal nanowires by self-assembly. - Angew. Chem. Int. Ed. 46 (2007) 7094-7097. doi: 10.1002/anie.200701613; Angew. Chem. 119 (2007) 7224-7227. doi: 10.1002/ange.200701613

[5] *JACS Select* is an online feature to showcase significant articles recently published in the JACS (https://pubsapp.acs.org:6443/JACSbeta/jvi/issues.html)

107. C. Loschen, S.T. Bromley, **K.M. Neyman**, F. Illas. Understanding ceria nanoparticles from first-principles calculations. - J. Phys. Chem. C 111 (2007) 10142-10145. doi: 10.1021/jp072787m

106. M. Bäumer, J. Libuda, **K.M. Neyman**, N. Rösch, G. Rupprechter, H.-J. Freund. Adsorption and reaction of methanol on supported palladium catalysts: Microscopic-level studies from ultrahigh vacuum to ambient pressure conditions. - Phys. Chem. Chem. Phys. 9 (2007) 3541-3558. doi:10.1039/b700365j

105. **K.M. Neyman**, K.H. Lim, Z.-X. Chen, L.V. Moskaleva, A. Bayer, A. Reindl, D. Borgmann, R. Denecke, H.-P. Steinrück, N. Rösch. Microscopic models of PdZn alloy catalysts: Structure and reactivity in methanol decomposition. - Phys. Chem. Chem. Phys. 9 (2007) 3470-3482. doi:10.1039/b700548b

104. S. González, **K.M. Neyman**, S. Shaikhutdinov, H.-J. Freund, F. Illas. On the promoting role of Ag in selective hydrogenation reactions over Pd-Ag bimetallic catalysts: A theoretical study. - J. Phys. Chem. C 111 (2007) 6852-6856. doi:10.1021/jp071584v

103. A.B. Mohammad, K.H. Lim, I.V. Yudanov, **K.M. Neyman**, N. Rösch. A computational study of H_2 dissociation on silver surfaces: The effect of oxygen in the added-row structure on Ag(110). - Phys. Chem. Chem. Phys. 9 (2007) 1247-1254. doi:10.1039/b616675j

102. C. Loschen, J. Carrasco, **K.M. Neyman**, F. Illas. First principles LDA+U and GGA+U study of cerium oxides: Dependence on the effective U-parameter. - Phys. Rev. B 75 (2007) 035115, 1-8; highly cited paper.[6] doi: 10.1103/PhysRevB.75.035115

101. **K.M. Neyman**, C. Inntam, L.V. Moskaleva, N. Rösch. Density functional embedded cluster studies of Cu_4, Ag_4 and Au_4 species interacting with oxygen vacancies on the MgO(001) surface. - Chem. - Eur. J. 13 (2007) 277-286. doi:10.1002/chem.200600545

2006

100. K.H. Lim, **K.M. Neyman**, N. Rösch. Destabilization of adsorbed CO on the Pd(111) surface by subsurface carbon: Density functional studies. - Chem. Phys. Lett. 432 (2006) 184-189.

99. D. Torres, **K.M. Neyman**, F. Illas. Oxygen atoms on the (111) surface of coinage metals: On the chemical states of the adsorbate. - Chem. Phys. Lett. 429 (2006) 86-90.

98. K.H. Lim, Z.-X. Chen, **K.M. Neyman**, N. Rösch. Comparative theoretical study of formaldehyde decomposition on PdZn, Cu and Pd surfaces. - J. Phys. Chem. B 110 (2006) 14890-14897.

97. I.V. Yudanov, **K.M. Neyman**, N. Rösch. C-O bond scission in methoxide on Pd nanoparticles: A density functional study. - Phys. Chem. Chem. Phys. 8 (2006) 2396-2401.

96. D. Torres, S. González, **K.M. Neyman**, F. Illas. Adsorption and oxidation of NO on Au(111) surface: Density functional studies. - Chem. Phys. Lett. 422 (2006) 412-416.

95. C. Di Valentin, **K.M. Neyman**, T. Risse, M. Sterrer, E. Fischbach, H.-J. Freund, V.A. Nasluzov, G. Pacchioni, N. Rösch. Density-functional model cluster studies of EPR g tensors of F_s^+ centers on the surface of MgO. - J. Chem. Phys. 124 (2006) 044708, 1-7.

94. K.H. Lim, Z.-X. Chen, **K.M. Neyman**, N. Rösch. Adsorption of acrolein on single-crystal surfaces of silver: Density functional studies. - Chem. Phys. Lett. 420 (2006) 60-64.

93. C. Inntam, L.V. Moskaleva, I.V. Yudanov, **K.M. Neyman**, N. Rösch. Adsorption of Cu_4, Ag_4 and Au_4 particles on regular MgO(001) surface: A density functional study using embedded cluster models. - Chem. Phys. Lett. 417 (2006) 515-520.

[6] Science Citation Index, Web of Science (WoS), 603 citations, accessed 8/4/2023.

92. A. Bayer, K. Flechtner, R. Denecke, H.-P. Steinrück, **K.M. Neyman**, N. Rösch. Electronic properties of thin Zn layers on Pd(111) during growth and alloying. - Surf. Sci. 600 (2006) 78-94.

91. C. Inntam, L.V. Moskaleva, **K.M. Neyman**, V.A. Nasluzov, N. Rösch. Adsorption of dimers and trimers of Cu, Ag, Au on regular sites and oxygen vacancies of the MgO(001) surface: a density functional study using embedded cluster models. - Appl. Phys. A 82 (2006) 181-189.

2005

90. **K.M. Neyman**, C. Inntam, A.V. Matveev, V.A. Nasluzov, N. Rösch. Single *d*-metal atoms on F_s and F_s^+ defects of MgO(001): A theoretical study across the periodic table. - J. Am. Chem. Soc. 127 (2005) 11652-11660.

89. **K.M. Neyman**, F. Illas. Theoretical aspects of heterogeneous catalysis: Application of density functional methods. - Catal. Today 105 (2005) 2-16.

88. **K.M. Neyman**, C. Inntam, A.B. Gordienko, I.V. Yudanov, N. Rösch. Adsorption of carbon on Pd clusters of nanometer size. A first-principles theoretical study. - J. Chem. Phys. 122 (2005) 174705, 1-9. Also selected for the May 16, 2005 issue of the Virtual Journal of Nanoscale Science & Technology.[7]

87. Z.-X. Chen, K.H. Lim, **K.M. Neyman**, N. Rösch. The effect of steps on the decomposition of CH_3O at PdZn alloy surfaces. - J. Phys. Chem. B 109 (2005) 4568-4574.

2004

86. Z.-X. Chen, K.H. Lim, **K.M. Neyman**, N. Rösch. Density functional study of methoxide decomposition on PdZn(100). - Phys. Chem. Chem. Phys. 6 (2004) 4499-4504.

85. **K.M. Neyman**, G.N. Vayssilov, N. Rösch. Transition metal clusters and supported species with metal-carbon bonds from first-principles quantum chemistry. - J. Organomet. Chem. 689 (2004) 4384-4394.

84. Z.-X. Chen, **K.M. Neyman**, K.H. Lim, N. Rösch. CH_3O decomposition on PdZn(111), Pd(111), and Cu(111). A theoretical study. - Langmuir 20 (2004) 8068-8077.

83. **K.M. Neyman**, R. Sahnoun, C. Inntam, S. Hengrasmee, N. Rösch. Computational study of model Pd-Zn nanoclusters and their adsorption complexes with CO molecules. - J. Phys. Chem. B 108 (2004) 5424-5430.

82. A. Föhlisch, F. Hennies, W. Wurth, N. Witkowski, M. Nagasono, M.N. Piancastelli, L.V. Moskaleva, **K.M. Neyman**, N. Rösch. Electronic structure and screening dynamics of ethene on single domain Si(001) from resonant inelastic X-ray scattering. - Phys. Rev. B 69 (2004) 153408, 1-4.

81. Z.-X. Chen, **K.M. Neyman**, N. Rösch. Theoretical study of segregation of Zn and Pd in Pd-Zn alloys. - Surf. Sci. 548 (2004) 291-300.

80. I.V. Yudanov, **K.M. Neyman**, N. Rösch. Density functional study of Pd nanoparticles with subsurface impurities of light element atoms. - Phys. Chem. Chem. Phys. 6 (2004) 116-123.[8]

79. **K.M. Neyman**, C. Inntam, V.A. Nasluzov, R. Kosarev, N. Rösch. Adsorption of *d*-metal atoms on the regular MgO(001) surface: Density functional study of cluster models embedded in elastic polarizable environment. - Appl. Phys. A 78 (2004) 823-828.

2003

[7] http://www.vjnano.org, covering a focused area of frontier research and published by the American Institute of Physics and the American Physical Society in cooperation with other societies and publishers.
[8] Ranked by the journal editor as being in the top 5% of all PCCP papers published in 2003/4, based on the number of citations till January 19, 2006. 99 ISI citations on 8/4/2023.

78. **K.M. Neyman**, D.I. Ganyushin, V.A. Nasluzov, N. Rösch, A. Pöppl, M. Hartmann. Electronic *g* values of Na^+-NO and Cu^+-NO complexes in zeolites: Analysis using a relativistic density functional method. - Phys. Chem. Chem. Phys. 5 (2003) 2429-2434.

77. Z.-X. Chen, **K.M. Neyman**, A.B. Gordienko, N. Rösch. Surface structure and stability of PdZn and PtZn alloys: Density functional slab model studies. - Phys. Rev. B 68 (2003) 75417, 1-8.

76. V.A. Nasluzov, V.V. Rivanenkov, A.M. Shor, **K.M. Neyman**, N. Rösch. Pd_3 and Pt_3 species on the α-Al_2O_3(0001) surface: Cluster models embedded in an elastic polarizable environment. - Chem. Phys. Lett. 374 (2003) 487-495. DOI:

75. V.V. Rivanenkov, V.A. Nasluzov, A.M. Shor, **K.M. Neyman**, N. Rösch. Adsorption of Pd and Pt atoms on α-Al_2O_3(0001) surface: Density functional studies of cluster models embedded in elastic polarizable environment. - Surf. Sci. 525 (2003) 173-183.

74. I.V. Yudanov, R. Sahnoun, **K.M. Neyman**, N. Rösch, J. Hoffmann, S. Schauermann, V. Johánek, H. Unterhalt, G. Rupprechter, J. Libuda, H.-J. Freund. CO adsorption on Pd nanoparticles: Density functional and vibrational spectroscopy studies. - J. Phys. Chem. B 107 (2003) 255-264.

2002

73. I.V. Yudanov, R. Sahnoun, **K.M. Neyman**, N. Rösch. Metal nanoparticles as models of single crystal surfaces and supported catalysts: Density functional study of size effects for CO on Pd(111). - J. Chem. Phys. 117 (2002) 9887-9896.

72. **K.M. Neyman**, D.I. Ganyushin, Ž. Rinkevičius, N. Rösch. Hydrogen-bonding effects on electronic *g*-tensors of semiquinone anion radicals. A relativistic density functional investigation. - Int. J. Quantum Chem. 90 (2002) 1404-1413.

71. **K.M. Neyman**, D.I. Ganyushin, A.V. Matveev, V.A. Nasluzov. Calculation of electronic *g*-tensors using a relativistic density functional Douglas-Kroll method. - J. Phys. Chem. A 106 (2002) 5022-5030.

70. V.A. Nasluzov, V.V. Rivanenkov, A.M. Shor, **K.M. Neyman**, U. Birkenheuer, N. Rösch. Density functional embedded cluster calculations on Lewis acid centers of the α-Al_2O_3 (0001) surface: Adsorption of a CO probe. - Int. J. Quantum Chem. 90 (2002) 386-402.

2001

69. V.A. Nasluzov, V.V. Rivanenkov, A.B. Gordienko, **K.M. Neyman**, U. Birkenheuer, N. Rösch. Cluster embedding in an elastic polarizable environment: Density functional study of Pd atoms adsorbed at oxygen vacancies of MgO(001). - J. Chem. Phys. 115 (2001) 8157-8171.

68. S.-H. Cai, **K.M. Neyman**, H. Knözinger, N. Rösch. Density functional model cluster study of adsorption of acetylene on magnesium oxide. - Surf. Sci. 479 (2001) 169-182. DOI:10.1016/S0039-6028(01)00974-8

2000 and before

67. S.-H. Cai, **K.M. Neyman**, A. Hu, N. Rösch. Tungsten atoms and clusters adsorbed on the MgO(001) surface: A density functional study. - J. Phys. Chem. B 104 (2000) 11506-11514.

66. J.F. Goellner, **K.M. Neyman**, M. Mayer, F. Nörtemann, B.C. Gates, N. Rösch. Ligand-free osmium clusters supported on MgO: a density functional study. - Langmuir 16 (2000) 2736-2743.

65. **K.M. Neyman**, N. Rösch, G. Pacchioni. Modification of structural and chemisorption properties of small palladium clusters supported on the MgO(001) surface from density functional calculations. - Appl. Catal. A 191 (2000) 3-13.

64. G.N. Vayssilov, M. Staufer, T. Belling, **K.M. Neyman**, H. Knözinger, N. Rösch. Density functional studies of alkali-exchanged zeolites. Cation location at six-rings of different aluminium content. - J. Phys. Chem. B 103 (1999) 7920-7928.

63. A.M. Ferrari, **K.M. Neyman**, M. Mayer, M. Staufer, B.C. Gates, N. Rösch. Faujasite-supported Ir_4 clusters: A density functional model study of metal-zeolite interactions. - J. Phys. Chem. B 103 (1999) 5311-5319.

62. A.M. Ferrari, C. Xiao, **K.M. Neyman**, G. Pacchioni, N. Rösch. Pd and Ag dimers and tetramers adsorbed at the MgO(001) surface: a density functional study. - Phys. Chem. Chem. Phys. 1 (1999) 4655-4661.

61. A. Hu, **K.M. Neyman**, M. Staufer, T. Belling, B.C. Gates, N. Rösch. A surface site as polydentate ligand of a metal complex: Density functional studies of rhenium subcarbonyls supported on magnesium oxide. - J. Am. Chem. Soc. 121 (1999) 4522-4523.

60. A.V. Matveev, **K.M. Neyman**, I.V. Yudanov, N. Rösch. Adsorption of transition metal atoms on oxygen vacancies and regular sites of the MgO(001) surface. - Surf. Sci. 426 (1999) 123-139.

59. **K.M. Neyman**, S. Vent, N. Rösch, G. Pacchioni. Transition metals supported on oxides: Density functional cluster studies of palladium deposition on MgO(001). - Topics Catal. 9 (1999) 153-161.

58. F. Illas, G. Pacchioni, A. Pelmenschikov, L.G.M. Pettersson, R. Dovesi, C. Pisani, **K.M. Neyman**, N. Rösch. Comment on "First principles determination of the bonding mechanism and adsorption energy for CO/MgO(001)". - Chem. Phys. Lett. 306 (1999) 202-204.

57. A.V. Matveev, **K.M. Neyman**, G. Pacchioni, N. Rösch. Density functional study of M_4 clusters (M = Cu, Ag, Ni, Pd) deposited on the regular MgO(001) surface. - Chem. Phys. Lett. 299 (1999) 603-612.

56. A.M. Ferrari, **K.M. Neyman**, T. Belling, M. Mayer, N. Rösch. Small platinum clusters in zeolites: Density functional study of CO adsorption on electronically modified models. - J. Phys. Chem. B 103 (1999) 216-226.

55. A.M. Ferrari, **K.M. Neyman**, S. Huber, H. Knözinger, N. Rösch. Density functional study of methane interaction with alkali and alkaline-earth metal cations in zeolites. - Langmuir 14 (1998) 5559-5567.

54. A.M. Ferrari, S. Huber, H. Knözinger, **K.M. Neyman**, N. Rösch. FTIR spectroscopic and density functional model cluster studies of methane adsorption on MgO. - J. Phys. Chem. B 102 (1998) 4548-4555.

53. I.V. Yudanov, S. Vent, **K. Neyman**, G. Pacchioni, N. Rösch. Adsorption of Pd atoms and Pd_4 clusters on the MgO(001) surface: A density functional study. - Chem. Phys. Lett. 275 (1997) 245-252.

52. A.M. Ferrari, **K.M. Neyman**, N. Rösch. CO interaction with alkali metal cations in zeolites: A density functional model cluster study. - J. Phys. Chem. B 101 (1997) 9292-9298.

51. I.V. Yudanov, V.A. Nasluzov, **K.M. Neyman**, N. Rösch. Density functional cluster description of ionic materials: Improved boundary conditions for MgO clusters with the help of cation model potentials. - Int. J. Quantum Chem. 65 (1997) 975-986.

50. J. Hahn, C.R. Landis, V.A. Nasluzov, **K.M. Neyman**, N. Rösch. Steric effects of the dinitrogen cleavage by three-coordinate molybdenum(III) complexes: A molecular mechanics study. - Inorg. Chem. 36 (1997) 3947-3951.

49. **K.M. Neyman**, V.A. Nasluzov, J. Hahn, C.R. Landis, N. Rösch. Density functional study of N_2 activation by Mo(III) complexes. Unusually strong relativistic effects in 4d-metal compounds. - Organometallics 16 (1997) 995-1000.

48. A.A. Voityuk, K. Albert, S. Köstlmeyer, V.A. Nasluzov, **K.M. Neyman**, P. Hof, R. Huber, M.J. Romão, N. Rösch. Prediction of alternative structures of the molybdenum site in the xanthine oxidase-related aldehyde oxido reductase. - J. Am. Chem. Soc. 119 (1997) 3159-3160.

47. **K.M. Neyman**, S. Vent, G. Pacchioni, N. Rösch. Adsorption of isolated Cu, Ni and Pd atoms on various sites of MgO(001): Density functional studies. - Nuovo Cimento della Societa Italiana di Fisica D 19 (1997) 1743-1748.

46. I. Yudanov, G. Pacchioni, **K. Neyman**, N. Rösch. Systematic density functional study of the adsorption of transition metal atoms on the MgO(001) surface. - J. Phys. Chem. B 101 (1997) 2786-2792.

45. **K.M. Neyman**, M. Staufer, V.A. Nasluzov, N. Rösch. Structure and vibrations of adsorption complexes NH_3/Ru(001): Density functional model cluster studies. - J. Mol. Cat. 119 (1997) 245-251.

44. K. Albert, **K.M. Neyman**, G. Pacchioni, N. Rösch. Electronic and geometric structure of bimetallic clusters: Density functional calculations on $[M_4\{Fe(CO)_4\}_4]^{4-}$ (M = Cu, Ag, Au) and $[Ag_{13}\{Fe(CO)_4\}_8]^{n-}$ (n = 0 - 5). - Inorg. Chem. 35 (1996) 7370-7376.

43. M. Staufer, **K.M. Neyman**, P. Jakob, V.A. Nasluzov, D. Menzel, N. Rösch. Density functional and infrared spectroscopy studies of bonding and vibrations of NH species adsorbed on the Ru(001) surface: A reassignment of the bending mode band. - Surf. Sci. 369 (1996) 300-312.

42. **K.M. Neyman**, V.A. Nasluzov, G.M. Zhidomirov. A density functional study of CO adsorption on three- and five-coordinate Al in oxide systems. - Catal. Lett. 40 (1996) 183-188.

41. A.L. Yakovlev, G.M. Zhidomirov, **K.M. Neyman**, V.A. Nasluzov, N. Rösch. Electron-deficient palladium clusters in zeolites and their complexes with probe CO molecules. A density functional model cluster study. - Ber. Bunsenges. Phys. Chem. 100 (1996) 413-417.

40. N. Rösch, **K.M. Neyman**, U. Birkenheuer, S. Krüger, V.A. Nasluzov. Density functional cluster and slab model studies of catalysis-relevant adsorption phenomena on metal and oxide surfaces. - Kinetika i Kataliz 37 (1996) 699-709 (Russ.); Kin. Catal. 37 (1996) 651-660 (Engl.).

39. A.L. Yakovlev, **K.M. Neyman**, G.M. Zhidomirov, N. Rösch. On the interaction of CO molecules with electron-deficient Pt atoms in zeolites: A density functional model cluster study. - J. Phys. Chem. 100 (1996) 3482-3487.

38. K. Albert, **K.M. Neyman**, V.A. Nasluzov, S.Ph. Ruzankin, C. Yeretzian, N. Rösch. On the electronic and geometric structure of bimetallic clusters. A comparison of the novel Na_6Pb cluster to Na_6Mg. - Chem. Phys. Lett. 245 (1995) 671-678.

37. **K.M. Neyman**, S.Ph. Ruzankin, N. Rösch. Adsorption of CO molecules on a MgO(001) surface. Model cluster density functional study employing a gradient-corrected potential. - Chem. Phys. Lett. 246 (1995) 546-554.

36. P. Strodel, **K.M. Neyman**, H. Knözinger, N. Rösch. Acidic properties of [Al], [Ga] and [Fe] isomorphously substituted zeolites. Density functional model cluster study of the complexes with a probe CO molecule. - Chem. Phys. Lett. 240 (1995) 547-552.

35. **K.M. Neyman**, P. Strodel, S.Ph. Ruzankin, N. Schlensog, H. Knözinger, N. Rösch. N_2 and CO molecules as probes of zeolite acidity: An infrared spectroscopy and density functional investigation. - Catal. Lett. 31 (1995) 273-285.

34. G. Pacchioni, **K.M. Neyman**, N. Rösch. CO adsorption on the (001) surface of MgO. A comparison of Hartree-Fock and local density functional results. - J. Electron Spectrosc. Relat. Phenom. 69 (1994) 13-21.

33. **K.M. Neyman**, N. Rösch. Structural and vibrational properties of Ni(111)/NO adsorption complexes: a LCGTO-LDF model cluster investigation. - Surf. Sci. 307/309 (1994) 1193-1199.

32. **K.M. Neyman**, N. Rösch, K.L. Kostov, P. Jakob, D. Menzel. Structural features of the NO/Ru(001) adsorption complexes: A linear combination of Gaussian-type orbitals local density functional model cluster analysis of high-resolution electron energy loss spectroscopy data. - J. Chem. Phys. 100 (1994) 2310-2321.

31. **K.M. Neyman**, N. Rösch. Bonding and vibrations of CO molecules adsorbed at transition metal impurity sites on the MgO(001) surface: A density functional model cluster study. - Chem. Phys. 177 (1993) 561-570.

30. **K.M. Neyman**, N. Rösch. Bonding and vibration of CO molecules adsorbed on low-coordinated surface sites of MgO: A LCGTO-LDF cluster investigation. - Surf. Sci. 297 (1993) 223-234.

29. **K.M. Neyman**, N. Rösch. Vibrational characteristics of adsorption complexes on the surface of ionic crystals: LCGTO-LDF cluster models of MgO/CO. - J. Mol. Struct. 293 (1993) 303-306.

28. **K.M. Neyman**, N. Rösch. Negatively charged μ_3-ON species on Ag(111): A LCGTO-LDF cluster analysis of HREELS data. - Surf. Sci. 287/288 (1993) 64-68.

27. **K.M. Neyman**, N. Rösch. Lateral interaction between adsorbates at ionic surfaces: Theoretical investigation of the CO vibrational frequency shift at MgO(001). - Ber. Bunsenges. Phys. Chem. 96 (1992) 1711-1715.

26. **K.M. Neyman**, N. Rösch. CO bonding and vibrational modes on a perfect MgO(001) surface: LCGTO-LDF model cluster investigation. - Chem. Phys. 168 (1992) 267-280.

25. V.A. Nasluzov, G.L. Gutsev, V.V. Rivanenkov, **K.M. Neiman**, A.G. Anshits. Using of the nonempirical pseudopotentials to impose boundary conditions on the MgO clusters. - Journal of Structural Chemistry 33 (1992) 157-161.

24. A.G. Anshits, E.N. Voskresenskaya, V.V. Rivanenkov, V.A. Nasluzov, **K.M. Neiman**. A DV Xα study of lithium-doped magnesium oxide. - React. Kinet. Catal. Lett. 46 (1992) 285-291.

23. V.V. Rivanenkov, V.A. Nasluzov, **K.M. Neyman**. Quantum-chemical investigation of effect of the adsorbed copper, silver and gold atoms on the electronic structure of the surface of the La_2CuO_4-type materials. - Sverhprovodimost (Superconduct.: Physics, Chemistry, Engineering, in russ.) 4 (1991) 1528-1532.

22. V.A. Nasluzov, **K.M. Neyman**, V.V. Rivanenkov, A.V. Kondratenko. Role of short-range interactions in formation of the electronic properties of the La_2CuO_4-type materials. – Sverhprovodimost (Superconduct.: Physics, Chemistry, Engineering, in russ.) 3 (1990) 185-193.

21. **K.M. Neiman**, A.V. Kondratenko, V.A. Nasluzov. Electronic structure, X-ray and X-ray photoelectron spectra of hexahalide complexes of platinum metals. - Koordinatsionnaya Khimiya 15 (1989) 1278-1285.

20. **K.M. Neiman**, A.V. Kondratenko, V.A. Nasluzov. Electronic structure and X-ray spectra of iron pentacarbonyl and hexacarbonyls of d metals as calculated by the Xα methods. - Koordinatsionnaya Khimiya 15 (1989) 383-388.
19. A.V. Kondratenko, E.S. Fomin, **K.M. Neiman**, V.A. Nasluzov. Electronic structure and X-ray spectra of the VO_4^{3-}, CrO_4^{2-}, MnO_4^{-} oxyanion isoelectronic series. - Optika i Spektroskpiya 66 (1989) 339-345.
18. V.A. Nasluzov, A.V. Kondratenko, **K.M. Neyman**, V.V. Rivanenkov. Structure of the occupied valent electronic states of La_2CuO_4-based high-T_c superconducting materials. - Institute of Inorganic Chemistry, Preprint No. 89-06, Novosibirsk, USSR, 1989, 34 p.
17. P.V. Avramov, A.V. Kondratenko, S.Ph. Ruzankin, **K.M. Neyman**, G.M. Zhidomirov. Ab initio quantum-chemical study of vacant electronic states of nd-metal oxides. 1.High-temperature superconductors on the La_2CuO_4 base. - Institute of Inorganic Chemistry, Preprint No. 89-05, Novosibirsk, USSR, 1989, 66 p.
16. A.V. Kondratenko, **K.M. Neiman**, G.L. Gutsev, G.M. Zhidomirov, S.Ph. Ruzankin. Quantum chemistry and spectroscopy of highly excited states of coordination compounds. - Journal of Structural Chemistry 29 (1988) 899-910.
15. V.A. Nasluzov, A.V. Kondratenko, **K.M. Neiman**, L.N. Mazalov. Electronic structure and the X-ray and photoelectron spectra of hexacyano-complexes of Fe(II) and Fe(III) in the cluster approximation by the SCF-Xα-SW method. - Journal of Structural Chemistry 29 (1988) 391-400.
14. V.A. Nasluzov, A.V. Kondratenko, **K.M. Neyman**, G.L. Gutsev. An Xα-DV study of the electronic structure, X-ray and X-ray photoelectron spectra of 3d metal cyanide complexes. - Chem. Phys. Lett. 146 (1988) 253-258.
13. V.A. Naslusov, A.V. Kondratenko, **K.M. Neyman**, L.N. Mazalov. An SCF Xα SW study of the electronic structure and X-ray and photoelectron spectra of Fe(II) and Fe(III) hexacyano complexes in a cluster approach. - Theoret. Chim. Acta 70 (1986) 429-441.
12. **K.M. Neiman**, A.V. Kondratenko, L.N. Mazalov, V.A. Nasluzov, P.V. Avramov. Electronic structure and the X-ray and photoelectron spectra of carbonyls of chromium, molybdenum and nickel. - Journal of Structural Chemistry 26 (1985) 851-857.
11. P.V. Avramov, A.V. Kondratenko, **K.M. Neiman**. Study of potential curves of ionized states of diatomic homonuclear molecules N_2 and F_2 by the self-consistent field Xα scattered wave method. - Journal of Structural Chemistry 26 (1985) 5-11.
10. **K.M. Neiman**, S.Ph. Ruzankin, A.V. Kondratenko, P.V. Avramov. Test calculations of permanganate ion by the Xα scattered wave method. - Journal of Structural Chemistry 25 (1984) 320-321.
9. A.V. Kondratenko, **K.M. Neyman**, L.N. Mazalov, P.V. Avramov. Resonant emission in the X-ray emission spectra. - In: Rentgenovskaja spektroskopija tverdogo tela (X-ray spectroscopy of solids, in russ.). - Sverdlovsk, USSR, 1984, p. 45-50.
8. **K.M. Neiman**, A.V. Kondratenko, L.N. Mazalov, E.A. Kravtsova, L.V. Molchanova, V.A. Nasluzov. SCF Xα SW and X-ray spectral study of the electronic structure of K_2PdCl_4 and K_2PtCl_4. - Journal of Structural Chemistry 24 (1983) 597-605.
7. **K.M. Neiman**, A.V. Kondratenko, V.A. Nasluzov, L.V. Molchanova, P.V. Avramov. Approximation of frozen Xα orbitals in the theory of X-ray and electron spectra. - Journal of Structural Chemistry 23 (1982) 349-354.
6. A.V. Kondratenko, L.N. Mazalov, **K.M. Neiman**, B.A. Kornev. Re-emission transitions in X-ray spectra of molecules. - Optika i Spektroskopiya 50 (1981) 1163-1169.

5. A.V. Kondratenko, L.N. Mazalov, **K.M. Neyman**. An ab initio investigation of the inner shell excited states of the molecule Cl_2. - Theoret. Chim. Acta 54 (1980) 179-185.
4. A.V. Kondratenko, L.N. Mazalov, **K.M. Neiman**. X-ray absorption spectra of the SO_2 molecule as studied by the Hartree-Fock-Roothaan method. - Optika i Spektroskopiya 49 (1980) 488-492.
3. A.V. Kondratenko, L.N. Mazalov, **K.M. Neiman**. Ab initio study of the X-ray emission spectra of molecules by self-consistent field method. Limitations of the orbital model. - Optika i Spektroskopiya 48 (1980) 1072-1080.
2. A.V. Kondratenko, L.N. Mazalov, **K.M. Neiman**. Distribution of the oscillator strengths in the K-absorption spectra of the CO and N_2 molecules. - Journal of Structural Chemistry 20 (1979) 785-787.
1. A.V. Kondratenko, L.N. Mazalov, **K.M. Neiman**. Near-edge fine structure of X-ray absorption spectra of molecules. Diatomic molecules CO and N_2. - Journal of Structural Chemistry 20 (1979) 170-175.

Invited review articles in book collections

9. A. Bruix, **K.M. Neyman**. How to design models for ceria nanoparticles: challenges and strategies for describing nanostructured reducible oxides. In: *Computational Modelling of Nanoparticles*, Eds. S.T. Bromley, S.M. Woodley, Series: Frontiers of Nanoscience, Vol. 12: Elsevier, Oxford, 2019, p. 55-99. ISBN: 978-0-08-102232-0 https://doi.org/10.1016/B978-0-08-102232-0.00001-4
8. Y. Lykhach, O. Brummel, A. Bruix, S. Fabris, I. Matolínová, V. Matolín, **K.M. Neyman**, J. Libuda. Pt-CeO_2 catalysts for fuel cell applications: From surface science to electrochemistry. In: *Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry*, K. Wandelt (Ed.), vol. 2, p. 189-201, Elsevier, Oxford, 2018. eBook ISBN: 9780128098943, Book ISBN: 9780128097397
7. S.M. Kozlov, H.A. Aleksandrov, L.V. Moskaleva, M. Bäumer, **K.M. Neyman**. Chapter 7.18 - From static to reacting systems on transition-metal surfaces. In: *Comprehensive Inorganic Chemistry II: From Elements to Applications*, Eds. J. Reedijk, K. Poeppelmeier, Vol. 7: Surface Inorganic Chemistry and Heterogeneous Catalysis, Eds. R. Schlögl, J.W. Niemantsverdriet, Elsevier, Oxford, 2013, p. 475-503. doi: 10.1016/B978-0-08-097774-4.00733-6.
6. N. Rösch, V.A. Nasluzov, **K.M. Neyman**, G. Pacchioni, G.N. Vayssilov. Supported metal species and adsorption complexes on metal oxides and in zeolites: Density functional cluster model studies. In: Computational Material Science, Ed. J. Leszczynski, Theoretical and Computational Chemistry Series, Vol. 15, Elsevier, Amsterdam, 2004, p. 365-448.
5. N. Rösch, A. Matveev, V.A. Nasluzov, **K.M. Neyman**, L. Moskaleva, S. Krüger. Quantum chemistry with the Douglas-Kroll-Hess approach to relativistic density functional theory: Efficient methods for molecules and materials. In: Relativistic electronic structure theory. Part II: Applications, Ed. P. Schwerdtfeger, Theoretical and Computational Chemistry Series, Vol. 14, Elsevier, Amsterdam, 2004, p. 656-722.
4. N. Rösch, G.N. Vayssilov, **K.M. Neyman**. Density functional model cluster studies of metal cations, atoms, complexes and clusters in zeolites. In: Host-guest-systems based on nanoporous crystals, Eds. F. Laeri, F. Schüth, U. Simon, M. Wark, Wiley-VCH, Weinheim, 2003, p. 339-357.
3. **K.M. Neyman**, G. Pacchioni, N. Rösch. Adsorption complexes on oxides: Density functional model cluster studies. In: Recent developments and applications of modern density functional theory, Ed. J.M. Seminario, Theoretical and Computational Chemistry Series, Vol. 4, Elsevier, Amsterdam, 1996, p. 569-619.
2. **K.M. Neyman**. Angewandte Quantenchemie und molekulare Simulation in der Katalyse, Status paper, DECHEMA e.V., Frankfurt/Main, 1995, p. 5-34.
1. N. Rösch, **K.M. Neyman**, U. Birkenheuer. Density functional investigations of adsorption at metal oxide surfaces. In: Adsorption on ordered surfaces of ionic solids and thin films, Eds. H.-J. Freund and E. Umbach, Springer Series in Surface Sciences, Vol. 33, Springer-Verlag, Berlin, 1993, p. 206-218.

Book

A.V. Kondratenko, **K.M. Neyman**. Quantum chemistry and spectroscopy of highly excited states. Coordination compounds of transition metals. Novosibirsk, Nauka, 1990. - 245 p.

Other publications

13. I. Khalakhan, L. Vega, M. Vorokhta, T. Skála, F. Viñes, Y.V. Yakovlev, **K.M. Neyman**, I. Matolínová. Surface structural dynamics in bimetallic PtNi alloy catalyst under simulated operational conditions. - CERIC Highlights 2020, Trieste, Italy (2021). https://www.ceric-eric.eu/2021/02/26/investigation-on-the-structural-dynamic-of-bimetallic-ptni-alloy-catalyst-under-operational-conditions/
12. I. Khalakhan, L. Vega, M. Vorokhta, T. Skála, F. Viñes, Y.V. Yakovlev, **K.M. Neyman**, I. Matolínová. Surface structural dynamics in bimetallic PtNi alloy catalyst under simulated operational conditions. - Elettra Highlights 2019-2020, Trieste, Italy (2020), p.118-119.
11. **K.M. Neyman**. Enabling catalysts to better clean car polluted air. - Highlights, ICREA Memoir 2018, https://www.icrea.cat/en/researcher/neyman/memoir-highlight-307488
10. **K.M. Neyman**. How nanoparticles give electrons away. - Highlights, ICREA Memoir 2016, https://www.icrea.cat/en/researcher/neyman/memoir-highlight-246995
9. Y. Lykhach, S.M. Kozlov, T. Skála, A. Tovt, V. Stetsovych, N. Tsud, F. Dvořák, V. Johánek, A. Neitzel, J. Mysliveček, S. Fabris, V. Matolín, **K.M. Neyman**, J. Libuda. Counting electrons on supported nanoparticles. - Elettra Highlights 2015-2016, Trieste, Italy (2016), p. 23-24.
8. **K.M. Neyman**. Teamwork between tiny catalyst nanoparticles. - Highlights, ICREA Memoir, 2011.
7. G.N. Vayssilov, Y. Lykhach, A. Migani, T. Staudt, G.P. Petrova, N. Tsud, T. Skála, A. Bruix, F. Illas, K.C. Prince, V. Matolín, **K.M. Neyman**, J. Libuda. Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. - Elettra Highlights 2010-2011, Trieste, Italy (2011), p. 74-75.
6. **K.M. Neyman**. Control of greenhouse gases and catalysis: Role of supercomputing. – Teraflop, Revista del CESCA, Barcelona, 94 (2007) 7.
5. **K.M. Neyman**. Quantum chemistry of surface complexes on oxides and transition metals, Habilitation Thesis in Theoretical Chemistry, Technische Universität München, 2003.
4. **K.M. Neyman**. Review on the book by J. Cioslowski "Electronic Structure Calculations on Fullerenes and Their Derivatives", Oxford University Press, 1995, ISBN 0-19. - Nachrichten aus Chemie, Technik und Laboratorium, VCH-Weinheim, 1996.
3. P.V. Avramov, A.V. Kondratenko, S.F. Ruzankin, **K.M. Neyman**, G.M. Zhidomirov. Ab initio quantum-chemical study of vacant electronic states of nd-metal oxides. 1. High-temperature superconductors on the La_2CuO_4 base. - Preprint. Institute of Inorganic Chemistry, No 89-05, Novosibirsk, 1989, 66 pp.
2. **K.M. Neyman**. Xα-SW study of the electronic structure and X-ray and photoelectron spectra of *d*-metal compounds, PhD (Candidate of Sciences) Thesis, Institute of Inorganic Chemistry, USSR Academy of Sciences, Novosibirsk, 1986.
1. A.V. Kondratenko, **K.M. Neyman**, L.N. Mazalov, P.V. Avramov. Resonant emission in X-ray emission spectra. - In: Rentgenovskaya spectroskopia tverdogo tela (in Russian), Sverdlovsk, Institute of Chemistry, 1984, pp.45-50.

Short highlights, links to newsletters, etc.

https://www.lavanguardia.com/natural/20180529/443928785634/descubren-un-efecto-catalizador-que-reduce-la-emision-de-dioxido-de-carbono-de-los-coches.html

https://www.somma.es/articles/carriers-catalyst-particles-bystanders-or-active-players-after-all

https://www.ceric-eric.eu/2021/02/26/investigation-on-the-structural-dynamic-of-bimetallic-ptni-alloy-catalyst-under-operational-conditions/

https://www.nsktv.ru/news/technology/neytralizuyushchie_vrednye_vybrosy_katalizatory_razrabatyvayut_v_novosibirske/

http://catalysis.ru/news/detail.php?ID=38782

http://www.sbras.info/news/uchenye-iz-rossii-i-ispanii-sozdali-katalizator-dlya-snizheniya-urovnya-ugarnogo-gaza-pri-nizki

https://www.interfax-russia.ru/siberia/news/novosibirskie-i-ispanskie-uchenye-sozdali-katalizator-dlya-snizheniya-urovnya-ugarnogo-gaza-pri-nizkih-temperaturah

https://newsib.net/tekhnologii/novosibirskie-uchyonye-razrabotali-unikalnyj-katalizator-dlya-snizheniya-ugarnogo-gaza.html?utm_source=yxnews&utm_medium=desktop

https://phys.org/news/2021-02-important-toxic-molecules-air-temperatures.html

https://www.pressetext.com/news/neuer-kat-funktioniert-auch-bei-minusgraden.html

https://www.miragenews.com/important-steps-for-transforming-toxic-518908/

https://www.technologynetworks.com/tn/news/tackling-vehicle-emissions-at-low-temperatures-346046

https://noticiasdelaciencia.com/art/41151/transformar-las-moleculas-toxicas-del-aire-a-bajas-temperaturas

https://nuestroclima.com/moleculas-toxicas-del-aire-transformadas-en-bajas-temperaturas/

https://www.eurekalert.org/pub_releases/2021-02/uob-isf022521.php

https://all-andorra.com/a-collaboration-between-the-university-of-barcelona-and-the-russian-academy-of-sciences-opens-the-way-for-reducing-emissions-of-automotive-pollutants/

https://www.alphagalileo.org/en-gb/Item-Display/ItemId/205066?returnurl=https://www.alphagalileo.org/en-gb/Item-Display/ItemId/205066

https://www.alphagalileo.org/en-gb/Item-Display/ItemId/205065?returnurl=https://www.alphagalileo.org/en-gb/Item-Display/ItemId/205065

https://www.iqtc.ub.edu/news/co-oxidation-activity/

https://www.ub.edu/web/ub/ca/menu_eines/noticies/2021/02/035.html

https://www.ub.edu/web/ub/es/menu_eines/noticies/2021/02/035.html

https://www.ub.edu/web/ub/en/menu_eines/noticies/2021/02/035.html

Articles received 100 or more ISI citations[9]

1. Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. *Nature Mater.* 10 (2011) 310 – ***827 citations***
2. First principles LDA+U and GGA+U study of cerium oxides: Dependence on the effective U-parameter. *Phys. Rev. B* 75 (2007) 035115 – ***715 citation*s**
3. Counting electrons on supported nanoparticles. *Nature Mater*. 15 (2016) 284 – ***585 citations***
4. Maximum noble-metal efficiency in catalytic materials: Atomically dispersed surface platinum. *Angew. Chem. Int. Ed*. 53 (2014) 10525 – ***428 citations***
5. Reassignment of the vibrational spectra of carbonates, formates, and related surface species on ceria: A combined density functional and infrared spectroscopy investigation. *J. Phys. Chem. C* 115 (2011) 23435 – ***367 citations***
6. CO adsorption on Pd nanoparticles: Density functional and vibrational spectroscopy studies. *J. Phys. Chem. B* 107 (2003) 255 – ***288 citation*s**
7. Systematic density functional study of the adsorption of transition metal atoms on the MgO(001) surface. *J. Phys. Chem. B* 101 (1997) 2786 – ***272 citations***
8. Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. *J. Mater. Chem*. 20 (2010) 10535 – ***204 citations***
9. Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. *Chem. Commun*. 46 (2010) 5936 – ***176 citations***
10. Adsorption of transition metal atoms on oxygen vacancies and regular sites of the MgO(001) surface. *Surf. Sci.* 426 (1999) 123 – ***167 citations***
11. The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation. *Nature Mater*. 17 (2018) 519 – ***165 citations***
12. CH_3O decomposition on PdZn(111), Pd(111), and Cu(111). A theoretical study. *Langmuir* 20 (2004) 8068 – ***159 citations***
13. Can the state of platinum species be unambiguously determined by the stretching frequency of adsorbed CO probe molecule? *Phys. Chem. Chem. Phys*. 18 (2016) 22108-22121 – ***144 citations***
14. Metal nanoparticles as models of single crystal surfaces and supported catalysts: Density functional study of size effects for CO on Pd(111). *J. Chem. Phys.* 117 (2002) 9887 – ***142 citations***
15. Methane activation by platinum: Critical role of edge and corner sites of metal nanoparticles. *Chem. - Eur. J*. 16 (2010) 6530 – ***138 citations***
16. Surface structure and stability of PdZn and PtZn alloys: Density functional slab model studies. *Phys. Rev. B* 68 (2003) 75417 – ***134 citations***
17. Density functional studies of model cerium oxide nanoparticles. *Phys. Chem. Chem. Phys*. 10 (2008) 5730 – ***132 citations***
18. On the promoting role of Ag in selective hydrogenation reactions over Pd-Ag bimetallic catalysts: A theoretical study. *J. Phys. Chem. B* 111 (2007) 6852 – ***130 citations***
19. Formation of superoxide anions on ceria nanoparticles by interaction of molecular oxygen with Ce^{3+} sites. *J. Phys. Chem. C* 115 (2011) 5817 – ***127 citations***
20. Silver residues as a possible key to remarkable oxidative catalytic activity of nanoporous gold. *Phys. Chem. Chem. Phys*. 13 (2011) 4529 – ***125 citations***

[9] Search of https://www.webofknowledge.com 7/10/2025 for Author=(Neiman KM* OR Neyman K* NOT Gourin NOT Kolb NOT Parker NOT Olanczuk NOT Rogers NOT Gordon NOT Jenkins NOT Sundset NOT Bofill) NOT Publication Name=(abstr*)

21. Water chemistry on model ceria and Pt/ceria catalysts. *J. Phys. Chem. C* 116 (2012) 12103 – ***123 citations***
22. CO oxidation activity of Pt/CeO_2 catalysts below 0ºC: Platinum loading effects. *Appl. Catal. B: Environ.* 286 (2021) 119931 – ***114 citations***
23. Atomically dispersed Pd, Ni and Pt species in ceria-based catalysts: Principal differences in stability and reactivity. *J. Phys. Chem. C* 120 (2016) 9852– ***112 citations***
24. Towards stable single-atom catalysts: Strong binding of atomically dispersed transition metals on the surface of nanostructured ceria. *Catal. Sci. Technol*. 6 (2016) 6806– ***112 citations***
25. Approaching nanoscale oxides: Models and theoretical methods. *Chem. Soc. Rev*. 38 (2009) 2657 – ***111 citations***
26. Comparative theoretical study of formaldehyde decomposition on PdZn, Cu and Pd surfaces. *J. Phys. Chem. B* 110 (2006) 14890 – ***110 citations***
27. Cluster embedding in an elastic polarizable environment: Density functional study of Pd atoms adsorbed at oxygen vacancies of MgO(001). *J. Chem. Phys*. 115 (2001) 8157 – ***109 citations***
28. Adsorption and reaction of methanol on supported palladium catalysts: Microscopic-level studies from ultrahigh vacuum to ambient pressure conditions. *Phys. Chem. Chem. Phys*. 9 (2007) 3541 – ***106 citations***
29. Density functional study of Pd nanoparticles with subsurface impurities of light element atoms. *Phys. Chem. Chem. Phys*. 6 (2004) 116 – ***105 citations***
30. Microscopic models of PdZn alloy catalysts: Structure and reactivity in methanol decomposition. *Phys. Chem. Chem. Phys*. 9 (2007) 3470 – ***102 citations***
31. Understanding ceria nanoparticles from first-principles calculations. *J. Phys. Chem. C* 111 (2007) 10142 – ***101 citations***
32. Electronic properties of thin Zn layers on Pd(111) during growth and alloying. *Surf. Sci*. 600 (2006) 78 – ***101 citations***

16200 **GoogleScholar** citations, ***H-index*=68**

Selected invited talks and contributed presentations

Invited talks at international conferences and university seminars

166. Describing complex catalytic nanomaterials by DFT calculations. – Invited lecture, Christian-Albrechts-Universität zu Kiel, Kiel, Germany, July 15, 2026.

165. Computational modelling of single-atom surface sites on oxide and bimetallic catalytic nanomaterials. - Keynote lecture, 4th International Symposium on Single-Atom Catalysis (ISSAC-4), Singapore, August 4-7, 2025

164. Modelling of catalytic nanomaterials for CO oxidation at very low temperatures. - Invited lecture, International Workshop on Oxides for Energy Applications: Bridging Experiment and Theory to Understand Functionality, Zaragoza, Spain, June 30 - July 4, 2025

163. Computational design of catalytic nanomaterials for oxidative abatement of air pollutants at very low temperatures. - Invited lecture, 11th Intern. Conference on Advanced Materials & Nanotechnology, Christchurch, New Zealand, February 9-13, 2025

162. Quantifying interface effects in catalytic nanomaterials combining DFT modelling and experiments. - Invited lecture, School of Chemical Sciences, University of Auckland, New Zealand, February 7, 2025

161. Complexity of catalytic nanomaterials: DFT modelling versus experiment. - Invited lecture, Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, February 3, 2025

160. From CO on MgO to catalytic nanomaterials. - Invited lecture, International workshop "Twins in catalysis: Merging theory and experiment", Barcelona, Spain, November 21-22, 2024

159. Approaching complexity of catalytic nanomaterials by DFT calculations. - Invited lecture, Summer School, German project SPP2080 "Catalysts and reactors under dynamic conditions for energy storage and conversion", Barcelona, Spain, October 14-18, 2024

158. How oxide supports affect transition-metal particles in catalytic nanomaterials. - Invited lecture, MC7 Colloquium "Supported metal nano-particles and alloys for catalytic applications", 31st General Conference of the Condensed Matter Division of the European Physical Society, Braga, Portugal, September 2-6, 2024

157. How to give a good talk. - Invited lecture, Cluster of Excellence "Materials for Energy Conversion and Storage", Inst. of Materials Chemistry, TU Wien, Vienna, Austria, April 17, 2024

156. Approaching complexity of nanomaterials for catalysis by DFT modelling. - Invited lecture, Conference of the COST Action 18234, Vienna, Austria, April 3-5, 2024

155. Computational modelling of bimetallic nanoparticles. - Invited lecture, Cluster of Excellence "Materials for Energy Conversion and Storage", Institute of Materials Chemistry, TU Wien, Vienna, Austria, March 20, 2024

154. Quantifying interface effects in catalytic nanomaterials combining DFT modelling and experiments. - Invited lecture, 37th Workshop on Chemistry and Physics of Novel Materials, Schladming, Austria, February 4-9, 2024

153. Effects of oxide supports on transition-metal particles in catalytic nanomaterials. - Invited lecture (on-line), International workshop on Fundamental Principles of Catalysis, Skoltech, Moscow, Russia, November 27-28, 2023

152. DFT calculations of the chemical ordering in bimetallic nanocrystallites using a TOP method. - Invited lecture (on-line), Webinar of the MDPI journal "Metals", May 25, 2023

151. Quantifying metal/metal-oxide interface effects in catalysts by combining DFT modelling with experiments. - Invited lecture, CLINT-Collaborative Research Center CRC 1452 'Catalysis at Liquid Interfaces', Erlangen, Germany, April 20, 2023

150. Quantifying metal/metal-oxide interface effects in catalytic nanomaterials by combining DFT modelling with experiments. - Invited lecture, Technische Universität München, TUM School of Natural Sciences, Department of Chemistry, Garching, Germany, April 18, 2023

149. Surprising oxidation of platinum in sub-nano states: Insights from catalytic experiments and DFT modelling. - Invited lecture, Conference "Designing the Future: Electro-, Photo- and Thermo-chemical Water Splitting" of the COST Action 18234, Brussels, Belgium, February 20-22, 2023

148. *In-silico* designing bimetallic nanoparticles. - Invited lecture, 4th International Conference on Materials: Advanced and Emerging Materials, Barcelona, Spain, October 19-21, 2022

147. Computational modelling of bimetallic nanoparticles in catalysis. - Plenary lecture (on-line), VII International School-Conference for Young Scientists "Catalysis: from Science to Industry", Tomsk, Russia, October 11-15, 2022

146. Quantifying interface effects in catalysis combining computer modelling and experiment. - Invited lecture (on-line), 3rd Summer School "Colloid and interface research & innovations" of the project EXTREME, Varna, Bulgaria, July 9-11, 2022

145. Quantifying metal/metal-oxide interface effects in catalytic nanomaterials. - Keynote lecture, ZCAM-ASEVA Workshop Metal-Oxide Ultrathin Films and Nanostructures, Zaragoza, Spain, July 4-8, 2022

144. Ordering in bimetallic nanoparticles: Effects of environment. - EMMC-eSSENCE International meeting on "Multiscale modelling of materials and molecules", Uppsala, Sweden, June 1-3, 2022

143. Metal/metal-oxide interface effects in catalytic nanomaterials: Density functional modelling versus experiment. - Department of Physical Electronics, Tel Aviv University, Tel Aviv, Israel, May 9, 2022

142. Quantifying metal/metal-oxide interface effects in catalytic nanomaterials: Density functional modelling versus experiment. - Department of Materials Science and Engineering, TECHNION - Israel Institute of Technology, Haifa, Israel, May 8, 2022

141. DFT modelling of oxide-supported metal clusters and nanoparticles relevant to catalysis. - Invited lecture, Cluster-Surface Interaction workshop (CSI2022), Santa Margherita Ligure, Italy, April 1-4, 2022

140. *In-silico* design of bimetallic nanocrystallites to speed-up their manufacturing. - Invited lecture, "Smart Composites International School" (SCIS) and IV International Baltic Conference on Magnetism (IBCM-2021), Svetlogorsk, Russia, August 29 - Sept. 2, 2021

139. Metal/metal-oxide interface effects in nanomaterials for catalysis and energy technologies: DFT modelling versus experiment. - Plenary lecture, International Workshop "Colloid and interface research & innovations", Varna, Bulgaria, July 18-21, 2021

138. Bimetallic nanoalloys of Pt and Pd with Au, Ag and Cu: Chemical orderings and properties from DFT calculations combined with a topological approach. - Invited lecture (on-line), CECAM Workshop "Multi-approach modeling of alloy nanoparticles: from non-equilibrium synthesis to structural and functional properties", Lyon, France, July 7-9, 2021

137. Modelling of catalytic nanomaterials using Density Functional Theory. - Plenary lecture (on-line), VI International School-Conference for Young Scientists "Catalysis: from Science to Industry", Tomsk, Russia, October 6-10, 2020

136. DFT modelling of metal nanoparticles in catalysis - Invited talk, International Conference "New directions for modeling nanocrystal catalysts", Virtual meeting of the COST Action CA18234, July 7, 2020

135. Modelling nanocomposite materials for catalysis: from ceria to bimetallic crystallites. - Invited talk, International Conference on Computational Materials Science for Nanoscale Modelling, COST Action CA18234 meeting, Department of Physics "Ettore Pancini", University of Naples Federico II, Naples, Italy, February 11-13, 2020

134. Effects of oxide supports on metal particles in catalytic nanomaterials: Lessons from density-functional modelling. - Invited lecture, Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia, October 4, 2019

133. Interface effects with oxide supports on the structure and reactivity of metal particles relevant for catalysis. - Invited lecture, Symposium "Catalysis at Metal-Support Interfaces", 258th American Chemical Society National Meeting and Exposition, San Diego, USA, August 25-29, 2019

132. Computational modelling of ceria-based nanocomposite materials for catalysis. - Invited lecture, Symposium "Advances in catalysis with ceria and other reducible oxides", 258th American Chemical Society National Meeting and Exposition, San Diego, USA, August 25-29, 2019

131. Atomic ordering in large bimetallic particles from DFT+Topological calculations. - Lecture in invited format, Symposium A2 "Nano-alloys: Theory, synthesis and characterization", XXVIII International Materials Research Congress, Cancun, Mexico, August 18-23, 2019

130. Metal/metal-oxide interface effects in catalytic nanomaterials: Theory versus experiment. - Invited lecture, Symposium B7 "Advanced Catalytic Materials: Nano and Bulk", XXVIII International Materials Research Congress, Cancun, Mexico, August 18-23, 2019

129. *In-silico* design of bimetallic nanocrystals. - Invited lecture, Faculty of Chemistry and Pharmacy, University of Sofia, Sofia, Bulgaria, May 28, 2019

128. Effects of oxide supports on reactivity of metal particles in catalysis and energy technologies. - Invited lecture, World Chemistry Forum (WCF) 2019, Barcelona, Spain, May 22-24, 2019

127. Metal/metal-oxide interface effects in catalytic materials: Theory versus experiment. - Invited lecture, Institute of Catalysis and Petroleum Chemistry, CSIC, Madrid, Spain, April 11, 2019

126. Interface effects with oxide supports on the structure and reactivity of metal particles relevant for catalysis and energy technologies. - Invited lecture, CECAM Workshop "Modeling metal-based nanoparticles: environment and dynamical effects", Grenoble, France, December 3-5, 2018

125. Computational modelling of catalytic nanomaterials - as simple as possible, but not simpler. - Invited lecture, Catalysis Research Center and Physics Department, Technische Universität München, Garching/München, Germany, November 15, 2018

124. Modelling metal/metal-oxide interface effects in nanocomposite materials for catalysis and beyond. - Invited seminar, Institut de Química Teòrica i Computacional, University of Barcelona, Barcelona, Spain, September 18, 2018

123. Density-functional modelling of nanocomposite materials for catalysis and new energy technologies. - Plenary lecture, International Workshop "Advanced Materials", Duni, Bulgaria, September 11-14, 2018

122. Density functional studies of ceria-based nanostructures: Recent progress and challenges. – Invited lecture, IUVSTA-ASEVA workshop WS-86-ASEVA-28 "Physics and Chemistry of Nanoscale Oxide Systems", Ávila, Spain, July 1-6, 2018

121. Progress in density-functional modelling of ceria-based nanomaterials for single-atom catalysis. - Keynote lecture, 2nd International Symposium on Single-Atom Catalysis (ISSAC2), Beijing, China, June 15-18, 2018

120. Computational engineering of bimetallic nanomaterials. - Invited seminar, Institute of Inorganic Chemistry, Russian Academy of Sciences, Novosibirsk, Russia, April 17, 2018

119. Modelling catalytic nanomaterials - as simple as possible, but not simpler. - Invited seminar, Boreskov Institute of Catalysis, Russian Academy of Sciences, Novosibirsk, Russia, April 11, 2018

118. Computational engineering of bimetallic nanomaterials. - Invited seminar, Boreskov Institute of Catalysis, Russian Academy of Sciences, Novosibirsk, Russia, January 24, 2018

117. Computational engineering of bimetallic nanocrystals. - Keynote lecture, 3rd International Conference "Electronic Structure Theory for Accelerated Materials Design: New Tool for Materials Science", NUST "MISiS", Moscow, Russia, October 30-31, 2017

116. Computational design of advanced nanoalloy materials for catalysis and beyond. - Invited seminar, N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia, October 26, 2017

115. Modelling catalytic nanomaterials - as simple as possible, but not simpler. - Invited lecture, Tianjin University, Tianjin, P.R. China, September 21, 2017

114. *In-silico* engineering bimetallic nanocrystals. - Invited lecture, 8th International Conference on Theory of Atomic and Molecular Clusters (TAMC-VIII), Beijing, P.R. China, September 17-22, 2017

113. Efficient computational engineering of bimetallic nanocrystals. - Invited lecture, 33rd European Conference on Surface Science (ECOSS-33), Szeged, Hungary, August 27 - September 1, 2017

112. Computational design of advanced nanoalloy materials for catalysis and beyond. - Invited lecture, Symposium "Advances in Computational Catalysis", 254th American Chemical Society National Meeting and Exposition, Washington DC, USA, August 20-24, 2017

111. Computational modeling of catalytic metal/metal-oxide nanostructures. - Invited lecture, Symposium "Metal-Support Interactions in Catalysis: Modeling, Characterization, and Design", 254th American Chemical Society National Meeting and Exposition, Washington DC, USA, August 20-24, 2017

110. Density-functional modelling of ceria-based nanomaterials for catalysis and energy technologies. - Keynote lecture, Swedish Theoretical Chemistry Conference 2017 – Bridging gaps. Annual meeting of the Swedish Chemical Society, Theoretical Chemistry Section, Gothenburg, Sweden, August 16-18, 2017

109. Computational design of bimetallic nanocrystals. - Invited lecture, 4th Conference on Multiscale Modelling of Materials and Molecules, Uppsala, Sweden, June 12-14, 2017

108. Computational design of bimetallic nanocrystals for catalysis and beyond. - Invited seminar, Chalmers University of Technology, Gothenburg, Sweden, May 30, 2017.

107. Modelling catalytic nanomaterials - as simple as possible, but not simpler. - Invited lecture, Nizhniy Novgorod State University, Nizhniy Novgorod, Russia, May 25, 2017.

106. Computational engineering of bimetallic catalysts to speed-up their targeted manufacturing. - Invited lecture, III Russian Congress on Catalysis "Roskataliz-2017", Nizhny Novgorod, Russia, May 22-26, 2017

105. Modelling catalytic nanomaterials - as simple as possible, but not simpler. - Jubilee Professor lecture, Chalmers University of Technology, Gothenburg, Sweden, May 11, 2017.

104. Computational design of bimetallic nanocrystals. - Invited colloquium, Brookhaven National Laboratory, Upton, USA, March 20, 2017

103. Approaching complexity of nanomaterials for catalysis and energy technologies by density-functional modelling. - Department of Chemistry - Ångström Laboratory, Uppsala University, Uppsala, Sweden, February 17, 2017

102. *In-silico* engineering bimetallic nanocrystals. - Invited seminar, Department of Chemistry - Ångström Lab., Uppsala University, Uppsala, Sweden, February 10, 2017

101. Effect of ionic Pt on the reducibility of Pt/CeO_2 nanocomposites. - Invited lecture, Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany, January 30, 2017

100. Modelling catalytic nanomaterials - as simple as possible, but not simpler. - Invited lecture, *The eSSENCE of . . . Computational Chemistry & Physics*, CECAM program seminar series, Department of Theoretical Chemistry and Biology, Royal Institute of Technology (KTH), Stockholm, Sweden, January 27, 2017

99. Modelling catalytic nanomaterials - as simple as possible, but not simpler. - Invited lecture, *The eSSENCE of . . . Computational Chemistry & Physics*, CECAM program seminar series, Ångström Laboratory, Uppsala University, Uppsala, Sweden, January 26, 2017

98. Modelling of ceria-based nanocomposites: Recent progress. - Invited seminar, Department of Chemistry - Ångström Lab., Uppsala University, Uppsala, Sweden, January 12, 2017

97. Sophisticated computational design of bimetallic nanocrystallites. - Invited lecture, Joint 4th Energy Materials Workshop of the Thomas Young Centre and TOUCAN International Conference "Shaping Nanocatalysts", London, UK, December 14-16, 2016

96. Computational modelling of inorganic nanomaterials for catalysis and energy technologies. - Invited lecture, Workshop on "Advanced Functional Materials", Pravets, Bulgaria, October 14-16, 2016

95. Innovative computational design of advanced nanoalloy materials for catalysis and beyond. - Keynote lecture, X International Conference "Mechanisms of Catalytic Reactions", School-Symposium "Quantum-mechanical modeling of catalytic processes", Svetlogorsk, Russia, October 2-7, 2016

94. Computational design of advanced nanoalloy materials. - Invited lecture, Annual User Meeting of the Spanish Supercomputing Network (Red Española de Supercomputación), León, Spain, September 20, 2016

93. Progress in modelling of catalytic materials: Engineering of bimetallic nanocrystallites. - Invited lecture. 1st Symposium of the Research Unit NAGOCAT – Nanoporous Gold Catalysts (FOR2213), Delmenhorst (near Bremen), Germany, September 8-9, 2016

92. Theoretical modelling of catalytic materials and their reactivity: As simple as possible, but not simpler. - Invited lecture, funCOS, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany, July 29, 2016

91. Efficient *in-silico* design of advanced nanoalloy materials for catalysis and related applications. - Invited lecture, 16th International Congress on Catalysis (ICC-16), Beijing, P. R. China, July 3-8, 2016

90. Materials for single-atom catalysis based on nanostructured ceria: Density-functional modelling. - Keynote lecture, International Symposium on Single-Atom Catalysis (Satellite Meeting of the 16th International Congress on Catalysis), Dalian, P.R. China, June 30 - July 2, 2016

89. Computationally designed nanoparticles as advanced models of bimetallic catalysts. – Invited lecture, 16th International Conference on Theoretical Aspects of Catalysis (ICTAC-16), Zakopane, Poland, June 19-23, 2016

88. Theoretical modelling of catalytic materials: As simple as possible, but not simpler. - Invited lecture, Jagiellonian University, Cracow, Poland, June 17, 2016

87. As simple as possible, but not simpler: DFT modelling of nanostructures in catalysis and energy technologies. - Invited lecture, Thomas Young Centre, The London Centre for the Theory and Simulation of Materials, London, UK, October 30, 2015

86. Approaching complexity in heterogeneous catalysis by density-functional modelling. - Keynote lecture, XII European Congress on Catalysis (EuropaCat) "Catalysis: Balancing the use of fossil and renewable resources", Kazan, Russia, August 30 - September 4, 2015

85. As simple as possible, but not simpler: Density-functional modelling of metal nanoparticles in catalysis. - Invited lecture, CECAM Workshop "Modeling metal-based nanoparticles: toward realistic environments", CECAM-FR-GSO, CEMES, Toulouse, France, June 29 - July 1, 2015

84. Interactions of hydrogen with transition metal nanoparticles from first principles. – Invited lecture, 11th International Conference on Diffusion in Solids and Liquids (DSL-2015), Munich, Germany, June 22-26, 2015

83. Theoretical modelling in heterogeneous catalysis: As simple as possible, but not simpler. - Invited lecture, International Symposium on Frontiers in Computational Catalysis, Tsinghua University, Beijing, P.R. China, May 31-June 2, 2015

82. Metal-metaloxide nanostructures in catalysis and energy technologies from a viewpoint of density functional modelling. - Invited lecture, International FOXSI Symposium, SFB "Functional Oxide Surfaces and Interfaces (FOXSI)" http://foxsi.tuwien.ac.at/, Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria, May 11-13, 2015

81. Nanostructured metal oxides and transition metal nanoparticles interacting with oxide surfaces from density-functional modelling. - Invited lecture, CECAM Workshop "Emergent structural and electronic phenomena at interfaces of nanoscale oxides", CECAM-HQ-EPFL, Lausanne, Switzerland, April 8-10, 2015

80. Density-functional modelling of metal-metaloxide nanostructures for catalysis and energy technologies. - Invited lecture, Workshop "Catalysis Meets Sensing", Karlsruhe Institute of Technology, Germany, February 6, 2015

79. Towards more realistic density functional modelling of nanostructures relevant to heterogeneous catalysis. - Invited lecture, SFB "Functional Oxide Surfaces and Interfaces (FOXSI)", Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria, December 3, 2014

78. Towards realistic first-principles modelling of complexity in heterogeneous catalysis. - Invited lecture, International Conference "Molecular Complexity in Modern Chemistry", Moscow, Russia, September 13-19, 2014

77. First-principles studies of metal particles in catalysis. - Invited lecture, XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications, Girona, Spain, June 30 - July 3, 2014

76. First-principles modelling of complex nanostructures: From catalysis to energy technologies. - Invited lecture, CIC energiGUNE, Parque Tecnológico de Álava, Miñano, Spain, June 23, 2014

75. Density-functional studies in heterogeneous catalysis: Extended surfaces or nanoparticles? - Invited lecture, Symposium "Clusters in Catalysis", 247th National Meeting of the American Chemical Society, Dallas, USA, March 16-20, 2014

74. Density-functional modelling of CeO_2 nanoparticles. - Tsinghua University, International Symposium on Atomic Cluster Catalysis, Beijing, P. R. China, November 21-22, 2013

73. Density-functional modelling of mono- and bimetallic nanoparticles relevant to catalysis. - Invited lecture, China-Europe International Workshop on Alloy Nanoparticles, Beijing, P. R. China, November 18-21, 2013

72. Density-functional modelling of CeO_2 nanoparticles: Structure, oxygen mobility and interactions with adsorbed molecules and metal species. - Invited lecture, 7th International Conference on the Theory of Atomic and Molecular Clusters, Birmingham, UK, September 15-20, 2013

71. Density-functional studies of nanoscale materials: Towards more realistic models in catalysis and beyond. - Invited lecture, School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore, March 5, 2013

70. Recent progress in density functional studies of ceria-based nanostructures. – Invited lecture, Chemistry Department, Chair of Quantum Chemistry, St. Petersburg State University, St. Petersburg, Russia, October 23, 2012

69. Catalysis from first principles: Is it crucial to account for the effects of nanostructuring? – Keynote lecture, IX International Conference "Mechanisms of Catalytic Reactions" (MCR-2012), St. Petersburg, Russia, October 22-25, 2012

68. Density functional studies of ceria nanostructures relevant for catalysis and beyond. – Invited talk, CECAM (ZCAM) Workshop "Modelling realistic inorganic nanostructures: Bridging the gap between theory and experiment", Zaragoza, Spain, September 5-7, 2012

67. First-principles modelling of nanostructures in catalysis and energy technologies. – Invited lecture, Workshop "In situ spectroscopy and model catalysis", Satellite of the 15th International Congress on Catalysis, Kloster Andechs / Munich, Germany, July 7, 2012

66. Density functional studies of ceria nanostructures relevant for catalysis and beyond. - Invited lecture, Department of Surface and Plasma Science, Charles University in Prague, Prague, Czech Republic, May 9, 2012

65. Modelling of ceria nanostructures relevant for catalysis. - Invited lecture. Catalysis Research Centre, Technische Universität München, Garching, Germany, November 10, 2011

64. First-principles modelling of nanostructures in catalysis. - Invited lecture, Department Chemie und Pharmazie, Graduate School Molecular Science, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany, July 27, 2011

63. Density-functional studies of nanoscale materials: Towards realistic models in catalysis and related areas. - Invited lecture, Department of Physical Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel, May 23, 2011

62. Towards more realistic models of nanostructures in catalysis described from first principles. - Invited lecture, Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva, Israel, May 18, 2011

61. First-principles modelling of bimetallic nanostructures in catalysis. - Invited lecture, CECAM workshop on "Nanoscale alloys: From experiments and theories to quantitative modeling", Lausanne, Switzerland, September 13-16, 2010

60. Computations in heterogeneous catalysis: Towards more realistic models. - Invited lecture, Symposium "Heterogeneous Catalysis", 3rd EuCheMS Chemistry Congress "Chemistry - the Creative Force", Nürnberg, Germany, August 30 - September 2, 2010

59. Carbon deposits on Pd catalysts modeled by nanoparticles. - Invited talk, 240th National Meeting of the American Chemical Society, Boston, MA, USA, August 22-26, 2010

58. Modelling of mono- and bimetallic nanostructures relevant to catalysis. - Plenary lecture, 4th Humboldt Conference on Computational Chemistry, Varna, Bulgaria, July 15-19, 2010

57. Density-functional studies of hydrogen in mono- and bimetallic nanostructures of relevance for catalysis and beyond. - Invited lecture, International Conference on Diffusion in Solids and Liquids, Paris, France, July 5-7, 2010

56. Density-functional studies of nanoscale materials: Towards more realistic models in catalysis. - Invited Seminar, Faculty of Chemistry, University of Sofia and National Centre of New Materials UNION, Sofia, Bulgaria, May 10, 2010

55. Density-functional studies of conventional and more realistic nanoparticle models of metal catalysts: PdZn and beyond. - Invited Seminar, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, April 12, 2010

54. Recent progress in density-functional studies of moderately large cerium oxide nanoparticles. - Oral presentation, COST-D41 "Inorganic Oxide Surfaces and Interfaces" Meeting of the Working Groups 1 and 3, Munich, Germany, March 18-19, 2010

53. Clean and Pt-modified ceria films and nanoparticles: Growth, structure and reactivity. - COST-D41 "Inorganic Oxide Surfaces and Interfaces" Annual Meeting, Paris, France, October 22-24, 2009

52. Density functional studies of nanoscale materials: Towards realistic models of catalysts and beyond. - Invited talk, 2nd Asian Symposium on Advanced Materials, Shanghai, P. R. China, October 11-14, 2009

51. Towards realistic models of catalysts: Density functional studies of nanoscale materials. - Invited Seminar, Institute of Theoretical and Computational Chemistry, Nanjing University, Nanjing, P. R. China, October 8, 2009

50. Density-functional studies of nanostructures based on metal oxides. - Invited lecture, COST-D41 "Inorganic Oxide Surfaces and Interfaces" WG2 Meeting, Krakow, Poland, April 30 - May 2, 2009

49. Modelling ceria nanoparticles and extended surfaces with irregularities. - Invited talk, COST-D41 "Inorganic Oxide Surfaces and Interfaces" Meeting of the Working Group 1, Erlangen, Germany, April 16-18, 2009

48. Formation and characterization of carbon deposits on palladium catalysts: Density-functional studies on representative nanoparticles. - Invited lecture, International Workshop on Computational Catalysis, Catalysis Research Centre, TU München, Garching, Germany, January 7-9, 2009.

47. Density-functional studies of bimetallic nanostructures relevant to catalysis and beyond. - Invited lecture, International Workshop "Computational Nanoalloys", Pisa, Italy, September 21-24, 2008

46. Towards realistic models of catalysts: Density functional studies of nanoscale materials. - Keynote lecture, 12th International Conference on Theoretical Aspects of Catalysis, Varna, Bulgaria, June 25-29, 2008

45. Density functional modeling of nanomaterials: Beyond the approach of ideal surfaces in catalysis. - Invited lecture, International Conference "Functional Materials and Nanotechnologies", Riga, Latvia, April 1-4, 2008

44. Density functional studies of bimetallic nanosystems. - Invited talk, Symposium "Bimetallic nanosystems: Tuning chemical and physical properties", Annual Meeting of the German Physical Society, Berlin, Germany, February 25-29, 2008

43. Beyond the approach of single-crystal surfaces: Nanosized metal and oxide particles as realistic models of catalytic materials. - Invited talk, International Workshop “Towards Reality in Nanoscale Materials”, Levi, Finland, December 10-12, 2007

42. Control of greenhouse gases and catalysis. - Invited talk, Jornada Catalana de Supercomputación (JOCS'07), “Research Related to Climate Change”, Parc Científic de Barcelona, Universitat de Barcelona, Barcelona, Spain, September 27, 2007

41. Density functional studies of catalytic materials and processes on their surfaces: From single crystals to nanostructures as models. - Institut für Physikalische und Theoretische Chemie (invitation Prof. J. Libuda), Universität Erlangen-Nürnberg, Germany, August 7, 2007

40. Density functional study of NO oxidation on Au(111) surface and thin films. - Invited talk, International Workshop “Catalysis-related issues of supported gold species”, TU München, Munich, Germany, March 19, 2007

39. Acrolein hydrogenation on silver catalysts. - Talk at the working meeting, Department Chemie (Theoretische Chemie), TU München, Munich, Germany, December 5, 2006

38. Theoretical studies of ceria nanoparticles. - Invited talk, COST-D41 Meeting “Inorganic Oxide Surfaces and Interfaces”, Vienna, Austria, November 2-4, 2006

37. Using core-level ionization potentials to identify very small oxide-supported metal species. - Invited talk, International Workshop “Supported Metal Clusters”, TU München, Munich, Germany, July 6-7, 2006

36. Small transition metal particles supported on MgO. - Group seminar, Departament de Química Física, Universitat de Barcelona, Spain, December 13, 2005

35. Models of supported metal nanoparticles and their building blocks from first-principles quantum chemistry. - Invited lecture, International Workshop “Nanoparticles and Oxide Surfaces” organized by Fritz-Haber-Institut der MPG (Berlin), Schloß Ringberg, Germany, September 4-9, 2005

34. Theoretical models of supported transition metal nanoparticles and their building blocks. - Lecture at the Centre especial de Recerca en Química Teòrica, Parc Científic de Barcelona, Barcelona, Spain, May 25, 2005

33. Surface complexes of small transition metal particles on metal oxides: First-principles theoretical studies. - Invited lecture, Meeting of the COST D19/005/01 working group “Chemical Reactivity of Metal Oxide Nanostructures”, Torino, Italy, May 12-15, 2005

32. Adsorption of acrolein on Ag surfaces. Density functional study. - Chemistry Department (invitation Prof. R. M. Lambert), Cambridge University, Cambridge, United Kingdom, April 4, 2005

31. Quantum chemical calculations of EPR parameters. - Invited lecture, Fourth School on Electron Paramagnetic Resonance , Alicante, Spain, September 6-10, 2004

30. Quantum chemistry of supported transition metal particles. - Invited lecture, Workshop “Catalysis - Linking Theory and Experiments”, Technische Universität München, Munich, Germany, July 19, 2004

29. Quantum chemistry of transition metal clusters. - Invited lecture, International Workshop “Nanoporous Crystals”, Delmenhorst/Bremen, Germany, June 11-12, 2004

28. Quantum chemistry of catalytic materials and surface complexes. - Symposium “Theoretical Chemistry”, Universität Ulm, Ulm, Germany, June 1-2, 2004

27. Oxide-supported *d*-metal species: Adsorbed atoms as elementary building blocks. - Group seminar, Departament de Química Física, Universitat de Barcelona, February 18, 2004

26. Quantum chemistry of *d*-metal species deposited on oxides: From atoms to nanoclusters. - Invited lecture, Annual Meeting of the German Physical Society, Dresden, Germany, March 24-28, 2003

25. Quantum chemistry of model catalysts: From supported transition metal atoms to nanoparticles. - Keynote lecture, 9th International Conference on Theoretical Aspects of Catalysis, Zakopane, Poland, June 25-30, 2002

24. Density functional studies of supported model metal catalysts: From atoms to nanoparticles. - Condensed Matter and Materials Physics Group, Department of Physics & Astronomy (invitation Prof. A. Shluger), University College London, London, United Kingdom, November 23, 2001

23. Oxide-supported metal catalysts: From atoms to nanoparticles. – Dept. de Química Física (invitation Prof. F. Illas), Universitat de Barcelona, Barcelona, Spain, October 31, 2001

22. Density functional studies of supported model metal catalysts: From atoms to nanoparticles. - Departament de Quimica Fisica (invitation Prof. J. F. Sanz), University Sevilla, Sevilla, Spain, October 26, 2001

21. Supported model metal catalysts: From atoms to nanoparticles. - Symposium "New directions in theoretical chemistry", University Ulm, Ulm, Germany, July 17-18, 2001

20. Density functional studies of transition metal species supported on oxides. - Tagung SFB 338, Schloß Ringberg, Germany, June 19-21, 2000

19. Transition metal species supported on metal oxide surfaces and in zeolites: Density functional studies. - Institut für Physikalische und Theoretische Chemie (invitation Prof. H.-P. Steinrück), Universität Erlangen-Nürnberg, Germany, February 17, 2000

18. Density functional studies of adsorption complexes on metals and oxides. - Seminar SFB 294 ”Moleküle in Wechselwirkung mit Grenzflächen” (invitation Prof. D. Michel), Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany, July 15, 1998

17. Adsorption complexes on metals and oxides: DF cluster studies of bonding and vibrations. - Dipartimento di Chimica Inorganica, Chimica Fisica e Chimica dei Materiali (invitation Prof. A. Zecchina, Prof. P. Ugliengo), Universita di Torino, Italy, November 13, 1996

16. Density functional studies of adsorption complexes on oxides. – International Conference ”Reactivity of oxide materials. Theory and experiment”, Como, Italy, November 8-9, 1996

15. Density functional model cluster studies of adsorption complexes on metals and oxides. - Lehrstuhl für Theoretische Chemie (invitation Prof. L.S. Cederbaum), Universität Heidelberg, Germany, May 20, 1996

14. Density functional studies of adsorption complexes with zeolites. - 6. Wochenendseminar ”Hohlkörperkristall-Komposite als Funktionsmaterialien”, Universität Bremen, Worpswede, Germany, May 3-4, 1996

13. Density functional calculations of surface complexes on metal oxides and in zeolites. - Ruhr-Universität Bochum, Graduirtenkolleg ”Dynamische Prozesse an Festkörperoberflächen”, Bochum, Germany, November 21, 1995

12. Density functional studies of zeolite systems. - Institut für Angewandte und Physikalische Chemie (invitat. Prof. G. Schulz-Ekloff), Universität Bremen, Germany, October 13, 1995

11. Untersuchungen von Adsorptionskomplexen auf Oxid- und Metalloberflächen mit Dichte-funktional-Methoden. - 31. Symposium für Theoretische Chemie ”Elektronenstruktur-methoden für große Systeme”, Loccum, Germany, October 10-13, 1995

10. Density functional studies of probe molecules chemisorbed on ionic catalytic materials. - Workshop “Theory in Catalysis”, Bad Soden, Germany, October 18-20, 1994

9. LDF modeling of interactions of small molecules with zeolites. - Lehrstuhl für Theoretische Chemie, Technische Universität München, Munich, Germany, February 7, 1994
8. Adsorption of NO molecules on metal surfaces: LDF model cluster study. - SFB 338 Tagung, Filzmoos, Austria, October 11-13, 1993
7. Adsorption of NO molecules on metal surfaces: a LDF model cluster analysis of HREEL and IR spectroscopy data. - Lehrstuhl für Theoretische Chemie, Technische Universität München, Munich, Germany, August 9, 1993
6. Density functional investigations of adsorption at metal oxide sirfaces. - Workshop on ”Cluster approach to chemistry and physics of surfaces and interfaces”, Centre Europeen de Calcul Atomique et Moleculaire (CECAM), Orsay, France, April 5-8, 1993
5. Quantum-chemical cluster models of adsorption on ionic materials: CO on metal oxide surfaces. - P. Sabatier University (Inst. Prof. J.-P. Daudey), Toulouse, France, April 1, 1993
4. Oxygen-down orientation of NO molecules adsorbed on metal surfaces. - Physik Department (invitation Profs. W. Brenig, D. Menzel), TU München, Munich, Germany, February 24, 1993
3. Bonding and vibrations of CO molecules adsorbed on MgO surface. - Institut für Physikalische Chemie (invitation Prof. E. Knözinger), Universität Siegen, Germany, November 10, 1992
2. LCGTO-LDF chemisorption cluster models: vibrational characteristics of Ni/C_2H_4 and MgO/CO. - Workshop on “Cluster approach to chemistry and physics of surfaces and interfaces”, Centre Europeen de Calcul Atomique et Moleculaire (CECAM), Orsay, France, March 31 - April 4, 1992
1. Bonding and vibrations of CO adsorbed on MgO surface. - SFB 338 Seminar, Institut für Physikalische Chemie (invit. Prof. H. Knözinger), Universität München, March 25, 1992

Contributed presentations at conferences and invited talks given by co-authors (selection)

235. When nanoparticles are catalytically more selective than single-crystal surfaces: Pd single-atom alloy with Cu. - 39th European Conference on Surface Science (ECOSS2026), Oslo, Norway, August 31 - September 4, 2026

234. DFT studies of remarkably selective of single-atom alloy catalyst nanoparticles. - 20th Intern. Conference on Theoretical Aspects of Catalysis (ICTAC-20), Delft, Netherlands, July 6-10, 2026

233. When platinum becomes not noble: Platinum-oxide clusters supported on ceria. - 4th General Meeting of the COST Action CA21101 (COSY), "COnfined Molecular SYstems: from a new generation of materials to the stars", Madrid, Spain, April 27-29, 2026

232. When platinum metal is not noble: Platinum-oxide clusters supported on ceria. - 4th Intern. Conference on Fundamentals and Applications of Cerium Dioxide in Catalysis, Portorož, Slovenia, September 17-20, 2024

231. Quantifying elusive interface effects in catalytic nanomaterials combining DFT modelling and experiment. - 18th International Congress on Catalysis, Lyon, France, July 14-19, 2024

230. Effects of oxide supports on metal particles in catalytic nanomaterials. - Intern. Conference "Development of Nanostructured Materials through Computational Modelling" of the COST Action 18234, Haifa, Israel, July 17-19, 2023

229. Oxidation of platinum at sub-nano scale: Insights from catalytic experiments and DFT modelling. - IUVSTA-ZCAM Workshop "Metal-Oxide Ultrathin Films and Nanostructures: Experiment Meets Theory", Zaragoza, Spain, July 3-7, 2023

228. Nanoalloys of Pt and Pd with Au, Ag and Cu: DFT calculations combined with Topological approach. - Intern. Meeting on Nanoalloys (IMN 2023), Orleans, France, May 9-11, 2023

227. DFT prediction of unexpectedly easy oxidation of small Pt clusters. - 1st Symposium (virtual) of the Working Group 3 "Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale" of the COST Action 21101, December 19, 2022

226. Modelling chemical ordering in bimetallic nanoparticles: Effects of reactive environment. - International Workshop on Non-Equilibrium and Environment Effects on Nanoalloys, Paris, France, December 7-9, 2022

225. Computational modelling of ceria-supported platinum catalysts under reactive conditions: Global optimization and ab initio thermodynamics study. - Intern. Virtual Workshop "Catalysis for Water Splitting", COST Action 18234, annual meeting, September 21-22, 2021

224. Modelling of Pt/CeO_2 and Pt/ZrO_2-CeO_2 systems relevant for CO and NO oxidation. – Intern. Virtual Conf. on Science and Technology, Nakhon-Ratchasima, Thailand, August 6, 2021

223. Machine-learning assisted characterization of ceria-supported platinum catalysts under reactive conditions: Interface effects. - International Workshop "Colloid and interface research & innovations", Varna, Bulgaria, July 18-21, 2021

222. Accuracy and efficiency of bimetallic nanoalloys representations for training surrogate energy models. - International Workshop "Colloid and interface research & innovations", Varna, Bulgaria, July 18-21, 2021

221. Effects of metal-oxide interfaces: adsorption of probe molecules on ceria-supported metal particles. - International Workshop "Colloid and interface research & innovations", Varna, Bulgaria, July 18-21, 2021

220. Ceria-supported transition metal particles: Electronic structure, charge transfer and chemical properties – Internat. Conference on Theoretical Aspects of Catalysis (virtual), June 30, 2021.

219. Machine-learning assisted characterization of ceria-supported Pt_yO_x clusters under reactive conditions. – Internat. Conference on Theoretical Aspects of Catalysis (virtual), June 30, 2021

218. Exploring the chemical ordering problem in bimetallic nanoalloys: strengths and limitations of topological descriptors. - International Conference on Theoretical Aspects of Catalysis (virtual), June 30, 2021

217. CO_x species at ceria nanoparticles with single atoms of Pd and Ag: structures, energies, CO frequencies. – Intern. Conference on Theoretical Aspects of Catalysis (virtual), June 14, 2021

216. DFT modelling of structure and reducibility of cerium dioxide nanoparticles doped by zirconium. - International Symposium on the DFT Modelling of Materials Relevant for Water Splitting (virtual), Barcelona, Spain, December 11, 2020

215. Metal/metal-oxide interface effects in catalytic nanomaterials: Theory versus experiment. – Symposium "Advances in cluster beam deposition", Okinawa, Japan, October 20-25, 2019

214. CO oxidation on the model Pd-Au/HOPG catalysts: NAP XPS and MS study. - XI International Conference "Mechanisms of Catalytic Reactions", Sochi, Russia, October 7-11, 2019

213. Metal/metal-oxide interface effects in catalytic materials: Theory versus experiment. - XI Int. Conference "Mechanisms of Catalytic Reactions", Sochi, Russia, October 7-11, 2019

212. Unraveling the morphological and topological key aspects of metal nanoparticles stability. - Hands-on "DFT and beyond: High-throughput screening and big-data analytics, towards exascale computational materials science", Barcelona, Spain, August 26 - Sept. 6, 2019.

211. CO oxidation on the model Pd-Au/HOPG catalysts: NAP XPS and MS study. - Symposium A2 "Nano-alloys: Theory, synthesis and characterization", XXVIII International Materials Research Congress, Cancún, Mexico, August 18-22, 2019

210. Accuracy of the topological approach for nanoalloys: Case study of PtCu nanoparticles. - Symposium A2 "Nano-alloys: Theory, synthesis and characterization", XXVIII International Materials Research Congress, Cancún, Mexico, August 18-22, 2019

209. Atomic ordering in bimetallic Pd-Au nanoparticles: Computational study of Pd surface segregation in reactive environment. - Russian-German Seminar on Catalysis, Novosibirsk, Russia, June 23-26, 2019

208. Accuracy of the Topological Approach for nanoalloys: Case study of PtCu nanoparticles. - International Meeting on Nanoalloys 2019 (IMN 2019), Genova, Italy, June 4-7, 2019

207. Atomic ordering in large bimetallic particles from DFT+Topological calculations. - Oral, International Meeting on Nanoalloys 2019 (IMN 2019), Genova, Italy, June 4-7, 2019

206. Atomic arrangement of PtCu bimetallic nanoparticles determined using topological energy expressions. - International Workshop "Advanced Materials", Duni, Bulgaria, September 11-14, 2018

205. Nanoscale materials chemistry in ceria based catalysts. - 3rd International Conference on Fundamentals and Applications of Cerium Dioxide in Catalysis, Barcelona, Spain, June 25-27, 2018

204. Correlation between Pt states, oxygen mobility and catalytic activity in Pt/CeO_2 composites for low-temperature CO oxidation. - 3rd International Conference on Fundamentals and Applications of Cerium Dioxide in Catalysis, Barcelona, Spain, June 25-27, 2018

203. Density functional studies of ceria-based nanostructures for catalysis: Recent progress and challenges. - 3rd International Conference on Fundamentals and Applications of Cerium Dioxide in Catalysis, Barcelona, Spain, June 25-27, 2018

202. Oxide-based nanomaterials for fuel cell catalysis: The interplay between supported single Pt atoms and particles. - GeCats Infoday 2017 “Synchrotron Radiation and Neutrons for Catalysis and Materials Science”, DECHEMA, Frankfurt/Main, Germany, 2017

201. Catalysts and catalysis through methods on models. - Workshop on Advanced Materials, Pomorie, Bulgaria, 2017

200. Pt/CeO_2 catalysts for low-temperature CO oxidation: Elusive role of ionic Pt. - 8^{th} World Congress on Oxidation Catalysis, Cracow, Poland, 2017

199. Redox-mediated conversion of atomically dispersed platinum to sub-nanometer particles. - 33^{rd} European Conference on Surface Science (ECOSS-33), Szeged, Hungary, August 27 - September 1, 2017

198. How nanoscale metal-oxide boundaries activate micrometer-sized metal particles for CO oxidation via a long-range effect. - XIII European Congress on Catalysis (EuropaCat-2017), Florence, Italy, 2017

197. Activation of oxygen in the ceria lattice by incorporation of platinum in Pt/CeO_2 catalysts for low-temperature CO oxidation. - XIII European Congress on Catalysis (EuropaCat-2017), Florence, Italy, 2017

196. Density-functional modeling of materials for single-atom catalysis based on nanostructured ceria. - Symposium “Catalysis at the Sub-Nanometer Scale”, 254th American Chemical Society National Meeting and Exposition, Washington DC, USA, 2017

195. Metal-support interactions in heterogeneous catalysis and electrocatalysis. - 2nd International Conference on Applied Surface Science (ICASS), Dalian, P.R. China, 2017

194. Palladium species at stoichiometric and partially reduced ceria: a density functional study. - IV Scientific Conference “Boreskov Readings”, Novosibirsk, Russia, 2017

193. Long ranging metal-oxide boundary effect in catalytic CO oxidation on ZrO_2-supported Pd. - 30. Symposium on Surface Science (3S’17), St. Moritz, Switzerland, 2017

192. Final report on the Work package 2 “Computational modelling”. - Review meeting of the FP7 project ChipCAT “Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology”, Brussels, Belgium, 2016

191. Computational engineering of bimetallic nanocrystals with tailor-made atomic ordering. - 18th International Symposium on Small Particles and Inorganic Clusters (XVIII-ISSPIC), Jyväskylä, Finland, 2016

190. Progress report on the Work package 2 “Computational modelling”. - General Assembly meeting of the FP7 project ChipCAT “Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology”, Prague, Czech Republic, 2016

189. Low platinum group metal fuel cell catalysts: from surface science to in-situ spectroelectro-chemistry. - 115th General Assembly of the German Bunsen Society for Physical Chemistry (Bunsentagung 2016), Rostock, Germany, 2016

188. Modeling interactions of transition metals with ceria nanoparticles: applications for fuel cell technologies. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Osnabrück, Germany, 2016

187. Modelling of ceria-based nanostructures inspired by the Action CM1104. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Osnabrück, Germany, 2016

186. Metal-oxide interactions in Pt/CeO_2 catalysts and related phenomena. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Osnabrück, Germany, 2016

185. Recent progress in density functional studies of ceria-based nanostructures: Inspiration by experimentalists from Erlangen and Prague. - WG3 Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Poznan, Poland, 2015

184. Effect of charge transfer between $CeO_2(111)$ support and Pt nanoparticles on their properties. - 4th International Workshop “New trends in Computational Chemistry for Industry Applications”, Barcelona, Spain, 2015

183. A GGA+U DFT investigation of silver atom, trimer and tetramer supported by a nanosized particle $Ce_{21}O_{42}$. - XII European Congress on Catalysis (Europacat) “Catalysis: Balancing the use of fossil and renewable resources”, Kazan, Russia, 2015

182. Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. - International Workshop “Low-precious-metal-content catalysts for PEM fuel cells”, Dijon, France, 2015

181. Modeling interactions of transition metal species with ceria nanoparticles for applications in fuel cell catalysts. - International Workshop “Low-precious-metal-content catalysts for PEM fuel cells”, Dijon, France, 2015

180. Tuning Pt catalysts for fuel cells by metal-oxide interactions. - International Workshop “Low-precious-metal-content catalysts for PEM fuel cells”, Dijon, France, 2015

179. Computational studies of nanoparticulate models of catalysts in the ChipCAT project. - International Workshop “Low-precious-metal-content catalysts for PEM fuel cells”, Dijon, France, 2015

178. Computational modeling of nanostructured ceria for the rational design of catalytic materials. - 250th National Meeting of the American Chemical Society, Boston, USA, 2015

177. Atomically dispersed and oxide-supported platinum in fuel cell catalysis: from surface science to in-situ spectroelectrochemistry. - 3S15 28th Symposium on Surface Science (3S15), Les Arcs 1800, France, 2015

176. Combining theory and experiment for the rational design of nanostructured Pt-CeO_2 catalytic materials with maximum noble-metal efficiency. - Chemical Reactions at Surfaces (Gordon Research Seminar), Surface Science Techniques for Addressing Contemporary Issues, Ventura, USA, 2015

175. Theoretical study of the CO interactions with mononuclear platinum species supported on nanoparticulate ceria. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Universitat de Barcelona, Spain, 2014

174. Atomically dispersed M species (M = Pd, Ni, Cu) in ceria nanoparticles: Stability and red-ox processes. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Universitat de Barcelona, Spain, 2014

173. Origin, stability, and effect of atomically dispersed Pt on nanostructured catalytic Pt-CeO_2 materials with maximum noble-metal efficiency. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Universitat de Barcelona, Spain, 2014

172. CO adsorption on mononuclear platinum species supported on nanoparticulate ceria. - 248th National Meeting of the American Chemical Society, San Francisco, USA, 2014

171. Studies of nanostructuring effects on model catalysts. - Symposium “Clusters, nanoparticles and nanostructures in catalysis and beyond”, Barcelona, Spain, 2014

170. Density-functional modelling of metal nanoparticles relevant for catalysis. - Clusters 2014: Workshop on reactivity and catalysis of metallic nanoclusters, Esbo, Finland, 2014

169. Theoretical investigations of metal particles as potential PEMFC electrocatalysts. - Clusters 2014: Workshop on Reactivity and catalysis of metallic nanoclusters, Esbo, Finland, 2014

168. Modelling the effect of metal-support interactions in nanostructured heterogeneous catalysts based on Pt and CeO_2. - VI Conference in Education and Modeling in Basic Sciences, Universidad de Medellín, Medellín, Colombia, 2014

167. Progress in modelling of ionic metal species in CeO_2-based catalytic nanomaterials. - WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Charles University in Prague, Czech Republic, 2014

166. Relative stability of mononuclear platinum species supported on nanoparticulate ceria and adsorption of CO on them. - WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Charles University in Prague, Czech Republic, 2014

165. Substrate effects on Pt nanoparticles. Electronic and structural differences induced by CeO_2(111) and MgO(100) on ~1 nm Pt clusters. - WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Charles University in Prague, Czech Republic, 2014

164. Report on the activities of the Working Group 3 "Catalysis". - Evaluation Meeting of the COST-MP0903 Action "Nanoalloys as Advanced Materials", Santa Margherita Ligure, Italy, 2014

163. Geometric and electronic structure of Pd-based intermetallic nanoparticles. - 4th International Symposium of Intermetallic Compounds in Catalysis, Santa Margherita Ligure, Italy, 2014

162. Modeling of bimetallic and intermetallic nanoparticles containing Pd. - General Meeting of the COST-MP0903 Action "Nanoalloys as Advanced Materials", Santa Margherita Ligure, Italy, 2014

161. Progress report on the Work package 2 "Computational modelling". - General Assembly meeting of the FP7 project ChipCAT "Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology", Barcelona, Spain, 2014

160. Oxygen vacancy formation on steps on CeO_2(111). - General Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Uppsala, Sweden, 2013

159. Electronic structure and absolute energies of steps on CeO_2(111). - General Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Uppsala, Sweden, 2013

158. Substrate mediated diversity in Pt-CeO_2 interactions. - General Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Uppsala, Sweden, 2013

157. Ionic Pt-CeO_2 composites for fuel cells applications: Combined experimental and density-functional studies. - General Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Uppsala, Sweden, 2013

156. H ad- and absorption in supported on MgO and unsupported Pd nanoparticles: Is consideration of a substrate always a must? - International Summer School on Basic Concepts and First-Principles Computations for Surface Science: Applications in Chemical Energy Conversion and Storage, Norderney, Germany, 2013

155. Progress report on the Work package 2 "Computational modelling". - General Assembly meeting of the FP7 project ChipCAT "Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology", Trieste, Italy, 2013

154. H adsorption and absorption in Pd nanoparticles supported on MgO(100). - 3rd International Workshop "New Trends in Computational Chemistry for Industry Applications", University of Barcelona, Barcelona, Spain, 2013

153. Distinguishing different Pt sites in Pt/CeO_2 via CO adsorption: A DFT study. - WG1/WG3 Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, TU Vienna, Vienna, Austria, 2013

152. Steps on $CeO_2(111)$: Step energies, STM appearance, O vacancy formation. - WG1/WG3 Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, TU Vienna, Vienna, Austria, 2013

151. On the concept of ionic platinum species in catalytic materials based on $Pt\text{-}CeO_2$ nanocomposites. - WG1/WG3 Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, TU Vienna, Vienna, Austria, 2013

150. First-principles modelling of ceria-based nanostructures relevant for catalysis. - 1st General Assembly Meeting of the European FP7 Project ChipCAT, Charles University, Prague, Czech Republic, 2013

149. Pt-Ti nanoparticles for possible use as a PEMFC cathode. - Joint Working Group Meetings of the COST Action MP0903 “Nanoalloys as Advanced Materials: From Structure to Properties and Applications”, Antalya, Turkey, 2012

148. Comparison between Pd-based intermetallic compounds and bimetallic alloys using density functional methods. - Joint Working Group Meetings of the COST-MP0903 Action “Nanoalloys as Advanced Materials: From Structure to Properties and Applications”, Antalya, Turkey, 2012

147. Recent progress in density functional studies of ceria-based nanostructures. - General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Charles University in Prague, Czech Republic, 2012

146. Electronic structure and absolute energies of steps on $CeO_2(111)$. - CECAM (ZCAM) Workshop “Modelling realistic inorganic nanostructures; bridging the gap between theory and experiment”, Zaragoza, Spain, 2012

145. Realistic first-principles description of Pd nanoparticles applied in catalysis and energy technologies. - CECAM (ZCAM) Workshop “Modelling realistic inorganic nanostructures; bridging the gap between theory and experiment”, Zaragoza, Spain, 2012

144. O_2 activation by Ag impurities and CO oxidation on nanoporous gold. A computational study. - 15^{th} International Congress on Catalysis, Munich, Germany, 2012

143. CO induced reconstruction of PdZn surface alloys? - 15^{th} International Congress on Catalysis, Munich, Germany, 2012

142. Towards realistic models of nanostructures in catalysis described from first principles. - 15^{th} International Congress on Catalysis, Munich, Germany, 2012

141. First-principles modelling of catalytically relevant surface alloys: PdAg, PdAu and AuAg. - 2^{nd} International Symposium on Intermetallic Compounds in Methanol Steam Reforming, Munich, Germany, 2012

140. Arrangement of components in intermetallic PdZn films on Pd(111) modified by CO adsorption. - 2^{nd} International Symposium on Intermetallic Compounds in Methanol Steam Reforming, Munich, Germany, 2012

139. Structure and stability of PdAu bimetallic nanocrystallites under hydrogenation conditions: A DFT study. - 2^{nd} International Symposium on Intermetallic Compounds in Methanol Steam Reforming, Munich, Germany, 2012

138. Modification of palladium nanoparticles by the surface and subsurface H and C species. - HPC-Europa2 Transnational Access Meeting (TAM), Amsterdam, Netherlands, 2012

137. Geometric arrangement of components in bimetallic PdZn/Pd(111) surfaces modified by CO adsorption: DFT, PM IRAS, and TPD study. - International Training School on Nanoalloys (ISNA), Pisa, Italy, 2012

136. Realistic models of palladium nanoparticles for hydrogen storage. - International Training School on Nanoalloys (ISNA), Pisa, Italy, 2012

135. Interaction of H_2O with ceria and Pt/ceria model catalysts. - 76th Annual Meeting of the DPG (German Physical Society) and DPG Spring Meeting, Berlin, Germany, 2012

134. Progress in density functional studies of Pd-Zn and Au-Ag nanostructures. - Working Groups Meeting of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Limerick, Ireland, 2011

133. CH_xO and CH_x species (x = 1-3) on a palladium nanoparticle representing model catalysts. - 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Santiago de Compostela, Spain, 2011

132. Computational modeling of carbonates on ceria nanoparticle. - 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Santiago de Compostela, Spain, 2011

131. Study of the interaction of Pt_x species with oxidized and reduced CeO_2(111). - 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Santiago de Compostela, Spain, 2011

130. CH_xO and CH_x species (x = 1-3) on a palladium nanoparticle representing model catalysts. - Satellite Meeting for the WATOC 2011 Congress "Theoretical modelling of materials", Barcelona, Spain, 2011

129. Towards more realistic models of nanostructures in catalysis described from first principles. - Symposium "Frontiers in interface science - Theory and experiment" organized by the Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, 2011

128. Topographic and electronic properties of line defects in the CeO_2(111) surface - CECAM Workshop "Understanding Structure and Functions of Reducible Oxide Systems - A Challenge for Theory and Experiment", ZCAM, Zaragoza, Spain, 2011

127. What makes ceria nanoparticles much more reactive than extended structures. - CECAM Workshop "Understanding Structure and Functions of Reducible Oxide Systems - A Challenge for Theory and Experiment", ZCAM, Zaragoza, Spain, 2011

126. Model structures of stripes on CeO_2 (111) surface. - CECAM Workshop "Understanding Structure and Functions of Reducible Oxide Systems - A Challenge for Theory and Experiment", ZCAM, Zaragoza, Spain, 2011

125. Modelling the interactions of Pt species with ceria surfaces and their effects on ceria reducibility - CECAM Workshop "Understanding Structure and Functions of Reducible Oxide Systems - A Challenge for Theory and Experiment", ZCAM, Zaragoza, Spain, 2011

124. CH_xO and CH_x species (x = 1-3) on a palladium nanoparticle representing model catalysts. - International Workshop "New Trends in Computational Chemistry for Industry Applications", University of Barcelona, Barcelona, Spain, 2011

123. Effect of the metal-support interaction on Pt_x/CeO_2(111) systems. - International Workshop "New Trends in Computational Chemistry for Industry Applications", University of Barcelona, Barcelona, Spain, 2011

122. Theoretical studies of CO adsorption on PdZn surface alloys and induced structural modifications of the substrate. – 2nd Symposium of the Institut de Química Teòrica i Computacional (IQTC-UB), Universitat de Barcelona, Barcelona, Spain, 2011

121. What makes ceria nanoparticles much more reactive than extended structures. – 2nd Symposium of the Institut de Química Teòrica i Computacional (IQTC-UB), Universitat de Barcelona, Barcelona, Spain, 2011
120. PdZn nanoalloys for methanol steam reforming: PM-IRAS, XPS and DFT studies. - Joint Working Group Meetings of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Barcelona, Spain, 2011
119. Surface science and technological catalysis on PdZn nanoalloys. - Joint Working Group Meetings of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Barcelona, Spain, 2011
118. Theoretical studies of CO adsorption on PdZn surface alloys and induced structural modifications of the substrate. – Joint Working Group Meetings of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Barcelona, Spain, 2011
117. Surface structures of bimetallic nanoparticles supported on thin oxide films. – Joint Working Group Meetings of the COST-MP0903 Action "Nanoalloys", Barcelona, Spain, 2011
116. Silver residues as a possible key to a remarkable oxidative catalytic activity of nanoporous gold. – Joint Working Group Meetings of the COST-MP0903 Action "Nanoalloys", Barcelona, Spain, 2011
115. Density-functional studies of bimetallic nanostructures relevant for catalysis. – Scientific Kick-off Meeting of the COST-MP0903 Action "Nanoalloys", Genova, Italy, 2010
114. Density-functional studies of metal catalysts: towards nanostructured models. – Scientific Kick-off Meeting of the COST-CM0904 Action "Network for Intermetallic Compounds as Catalysts for Steam Reforming of Methanol", Berlin, Germany, 2010
113. Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. – Final Meeting of the COST-D41 Action "Inorganic Oxides: Surfaces and Interfaces", Turin, Italy, 2010
112. Chemistry of pure and Pt-loaded ceria surfaces: experiment and theory. – Final Meeting of the COST-D41 Action "Inorganic Oxides: Surfaces and Interfaces", Turin, Italy, 2010
110. What makes ceria nanoparticles much more reactive than extended structures. - COST-D41 "Inorganic Oxide Surfaces and Interfaces" Meeting of the Working Groups 1 and 3, Munich, Germany, 2010
109. DFT+U study of the interaction of Pt atoms with the regular CeO_2(111) surface. - COST-D41 "Inorganic Oxide Surfaces and Interfaces" Meeting of the Working Groups 1 and 3, Munich, Germany, 2010
108. Computational modeling of CO and CO_2 adsorption on defect ceria nanoparticles. – HCP Europa 2 Transnational Access Meeting, Montpellier, France, 2009
107. Interaction of atoms and small molecules on metal surfaces and nanoparticles. – 13th International Conference on the Applications of Density Functional Theory in Chemistry and Physics, DFT09, Lyon, France, 2009
106. Modeling NO_x storage and reduction catalysts – An overview. – Europacat IX, Salamanca, Spain, 2009
105. Mechanism of acrolein hydrogenation on silver catalysts: A density functional study. – VIII International Conference "Mechanisms of Catalytic Reactions", Novosibirsk, Russia, 2009
104. Density functional studies of model cerium oxide nanoparticles. – 13th International Congress of Quantum Chemistry, Helsinki, Finland, 2009
103. NSR model catalysts - An overview. – 42. Jahrestreffen Deutscher Katalytiker, Weimar, Germany, 2009

102. Modeling NO_x storage catalysts: An overview. – 6th International Workshop on Oxide Surfaces (IWOX-VI), Schladming, Austria, 2009

101. Modeling storage processes in heterogeneous catalysis: Adsorption and reaction of nitrogen oxides and sulfur oxides on oxide surfaces and oxide supported metal nanoparticles. – Annual Meeting of the COST-D41 Action "Inorganic Oxides: Surfaces and Interfaces", Barcelona, Spain, 2008

100. Nano-size crystallites as models for supported catalysts: Carbon subsurface formation and adsorption of NO on Pd nanoparticles. – Annual Meeting of the COST-D41 Action "Inorganic Oxides: Surfaces and Interfaces", Barcelona, Spain, 2008

99. Ceria: What we don't know (for sure). – Annual Meeting of the COST-D41 Action "Inorganic Oxides: Surfaces and Interfaces", Barcelona, Spain, 2008

98. Low-energy localized states of ceria nanoparticles computed using DFT+U and interatomic potential approaches. – Annual Meeting of the COST-D41 Action "Inorganic Oxides: Surfaces and Interfaces", Barcelona, Spain, 2008

97. Identification of IRAS signals using DFT calculations: Case study of NO adsorption on Pd nanoparticles. – 44th Symposium on Theoretical Chemistry, Ramsau, Austria, 2008

96. How C-O bond breaks during methanol decomposition on palladium nanocrystallites. – 12th International Conference on Theoretical Aspects of Catalysis, Varna, Bulgaria, 2008

95. DFT+U studies of cerium oxide nanoparticles: Modelling of adsorption. – COST-D41 Annual Meeting "Inorganic Oxide Surfaces and Interfaces", Berlin, Germany, 2007

94. Nanosized metal and oxide particles as realistic models of catalytic materials. – 43rd Symposium for Theoretical Chemistry, Saarbrücken, Germany, 2007

93. Acrolein hydrogenation on silver catalysts: A density functional study of mechanism. – The 234th ACS National Meeting, Boston, USA, 2007

92. Quantum chemical modelling of nanosized transition metal catalysts: Density functional calculations of Pd and Cu nanoclusters. – Russian-German Seminar on Catalysis "Bridging the Gap between Model and Real Catalysis", Altai Mountains, Russia, 2007

91. Sobre el mecanisme de formació de nanocables metàl.lics via autoensablatge (On the mechanism of metal nanowires formation by self-assembling). – XXIIIena Reunió de la Xarxa de Química Teòrica de Catalunya, Tarragona, Spain, 2007

90. Theoretical investigation of the properties of ceria and small ceria clusters. – Symposium on Theoretical Chemistry: Quantum Chemistry – Methods and Applications, Erkner / Berlin, Germany, 2006

89. Water gas shift reaction on supported ceria and ceria nanoclusters. – International Workshop "Supported Metal Clusters", TU München, Munich, Germany, 2006

88. Adsorption of small coinage metal particles on regular sites and oxygen vacancies of the MgO(001) surface: First-principles theoretical studies. – International Workshop "Supported Metal Clusters", TU München, Munich, Germany, 2006

87. Small supported metal particles as model catalysts. – 11th International Conference on Theoretical Aspects of Catalysis, Schmöckwitz/Berlin, Germany, 2006

86. Nanocluster modeling of Pd catalysts for methanol dehydrogenation: Mechanism of catalyst poisoning by carbonaceous species. – 11th International Conference on Theoretical Aspects of Catalysis, Schmöckwitz/Berlin, Germany, 2006

85. Adsorption of small coinage metal particles on regular sites and oxygen vacancies of the MgO(001) surface: First-principles theoretical studies. – International Conference on Clusters at Surfaces, Warnemünde, Germany, 2006

84. Activation of hydrogen on added-row reconstructed Ag(110)(n×1)O surface: A DFT slab model study. – 105. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Erlangen, Germany, 2006

83. Theoretical studies related to methanol steam reforming on Pd/ZnO catalysts. – 105. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Erlangen, Germany, 2006

82. Dehydrogenation of methanol on Pd nanoparticles: A DFT study of catalyst poisoning by carbonaceous species. – 105. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Erlangen, Germany, 2006

81. Methanol steam reforming on Pd/Zn/ZnO catalysts. – 105. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Erlangen, Germany, 2006

80. Partial oxidation of methanol on well-defined supported model catalysts. – 105. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Erlangen, Germany, 2006

79. First-principle modelling of surfaces and their reactivity. – Jornada Catalana de Supercomputació, Universitat Rovira i Virgili, Tarragona, Spain, 2005

78. Theoretical studies of advanced materials based on nanoparticles. – Jornada Catalana de Supercomputació, Universitat Rovira i Virgili, Tarragona, Spain, 2005

77. Theoretical studies of methanol steam reforming on Pd/ZnO catalyst. – Reporting Seminar, DFG Priority Program 1091 "From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis", Berlin, Germany, 2005

76. Synthesis and partial oxidation of methanol on well-defined model catalysts and single crystals. – Reporting Seminar, DFG Priority Program 1091 "From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis", Berlin, Germany, 2005

75. Density functional studies of adsorption and oxidation of NO on Au(111) surface and thin film. – 23th European Conference on Surface Science (ECOS 23), Berlin, Germany, 2005

74. Surface complexes of small transition metal particles on metal oxides: First-principles theoretical studies. – 89th International Bunsen Discussion Meeting "Chemical processes at oxide surface: from experiment to theory", Meschede, Germany, 2005

73. Theoretical studies of well-defined noble-metal model catalysts: Pd nanoclusters. – "Synthesis and partial oxidation of methanol on well-defined supported model catalysts", workshop in the frameworks of the DFG Priority Program 1091 "From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis", Fritz-Haber-Institut der MPG, Berlin, Germany, 2005

72. Acrolein and hydrogen adsorption on Ag surfaces. – Working meeting of cooperation partners, TU Darmstadt, Darmstadt, Germany, 2005

71. Calculation of EPR parameters using a relativistic density functional Douglas-Kroll-Hess method. Theory and applications. – Final Report Colloquium of the DFG Priority Program 1051 "High Field EPR in Biology, Chemistry and Physics", Hünfeld, Germany, 2005

70. Pd/Zn/ZnO catalysts for methanol steam reforming. – Reporting Seminar, DFG Priority Program 1091 "From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis", Berlin, Germany, 2004

69. Interactions with model supported catalysts. – Reporting Seminar, DFG Priority Program 1091 "From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis", Berlin, Germany, 2004

68. Transition metal clusters adsorbed on MgO(001) surface: Density functional study using embedding in elastic polarizable environment. – Status Seminar, DFG Priority Program 1153 “Clusters at Surfaces”, Bad Honnef, Germany, 2004

67. CH_3O decomposition on flat and stepped surfaces of PdZn alloy. – Status Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Erlangen, Germany, 2004

66. Density functional studies of paramagnetic surface centres and adsorption complexes on oxides. – Status Seminar, DFG Priority Program 1051 “High Field EPR in Biology, Chemistry and Physics”, Hirschegg, Austria, 2003

65. Calculation of EPR parameters using a relativistic density functional method based on the two-component Douglas-Kroll formalism. – Status Seminar, DFG Priority Program 1051 “High Field EPR in Biology, Chemistry and Physics”, Hirschegg, Austria, 2003

64. Pd/Zn/ZnO catalysts for methanol steam reforming. – Status Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Innsbruck, Austria, 2003

63. Interactions with model supported catalysts. – Status Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Innsbruck, Austria, 2003

62. Quantum chemistry of model catalysts: From supported *d*-metal atoms to nanoparticles. – EuropaCat-VI, Innsbruck, Austria, 2003

61. Density functional studies of PdZn alloys. – EuropaCat-VI, Innsbruck, Austria, 2003

60. DFT Study of Methanol Decomposition on Cu(111), Pd(111) and PdZn(111). – Status Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Erlangen, Germany, 2003

59. Theoretical studies of structure and segregation at the surfaces of Pd-Zn alloys. – XXXVI Annual Meeting of German Catalyst Chemists, Weimar, Germany, 2003

58. Density functional studies of *d*-metal species supported on oxides: From atoms to nano-particles. – 3rd International Workshop on Oxide Surfaces, Sapporo, Japan, 2003

57. Pd/Zn/ZnO catalysts for methanol steam reforming. – Reporting Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Berlin, Germany, 2002

56. Interactions with model supported catalysts. – Reporting Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Berlin, Germany, 2002

55. Transition metal atoms adsorbed on oxide surfaces: Systematic density functional study using EPE embedding. – EURESCO Conference on Fundamental Aspects of Surface Science “Structure and Reactivity of Oxide Surfaces”, Acquafredda di Maratea, Italy, 2002

54. Calculation of electronic g-tensors using a relativistic density functional Douglas-Kroll method. – Reporting Colloquium, DFG Priority Program 1051 “High Field EPR in Biology, Chemistry and Physics”, Berlin, Germany, 2002

53. Theoretical studies relevant to methanol steam reforming on Pd/Zn/ZnO catalysts. – Preparatory Meeting, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Erlangen, Germany, 2002

52. Density functional study of supported model metal catalysts: From atoms to nanoclusters – Annual Meeting of the German Physical Society, Regensburg, Germany, 2002

51. Density functional calculations of EPR g tensors using relativistic Douglas-Kroll formalism. – Priority Program 1051 of DFG, “High Field EPR in Biology, Chemistry and Physics”, Status Seminar, Berlin, Germany, 2001
50. Calculation of EPR g-tensors using a relativistic density functional method based on the two-component Douglas-Kroll formalism. – Specialized Colloque AMPERE “ESR and Solid State NMR in High Magnetic Fields”, Stuttgart, Germany, 2001
49. Partial oxidation of methanol on well-defined model catalysts. – Status Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Berlin, Germany, 2001
48. Methanol steam reforming on Pd/Zn/ZnO catalysts. – Status Seminar, DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Berlin, Germany, 2001
47. Partial oxidation of methanol on well-defined model catalysts. – Selection Colloquium of the DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Berlin, Germany, 2000
46. Methanol steam reforming on Pd/Zn/ZnO catalysts. – Selection Colloquium of the DFG Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Berlin, Germany, 2000
45. Formalism of EPR g-tensor calculations using density functional Douglas-Kroll method with self-consistent spin-orbit interactions. – Priority Program of DFG, “Hochfeld-EPR in Biologie, Chemie und Physik”, Berichtsolloquium, Königstein, Germany, 1999
44. Theoretical study of sodium interaction with six-membered zeolite rings of different aluminum content. – 32. Jahrestreffen deutscher Katalytiker, Friedrichroda, Germany, 1999
43. Density functional studies of alkali-exchanged zeolites. Framework basicity and Lewis acidity of the cations. – 11. Deutsche Zeolith-Tagung, Stuttgart, Germany, 1999
42. Density functional studies of metal species in zeolites. – DFG-Kolloquium “Nanoporöse Kristalle”, Bonn, Germany, 1998
41. Small platinum clusters in zeolites: Density functional study of CO adsorption on electronically modified models. – 10. Deutsche Zeolith-Tagung, Bremen, Germany, 1998
40. Density functional studies of metal species in zeolites. – DFG-Kolloquium “Nanoporöse Kristalle”, Bonn, Germany, 1996
39. Modellierung katalytisch relevanter Systeme. – Seminar “Wasserbasierte Metalkomplex-Katalysatoren”, Berlin, Germany, 1996
38. Electron-deficient metal particles in zeolites: A density functional cluster model study. – 6th International conference on theoretical aspects of heterogeneous catalysis, Tarragona, Spain, 1996
37. Density functional studies on the bonding and vibrations of nitrogen containing species on a Ru(001) surface. – 6th International conference on theoretical aspects of heterogeneous catalysis, Tarragona, Spain, 1996
36. Electron-deficient metal particles in zeolites. A density functional cluster study – 6th Intern. conference on theoretical aspects of heterogeneous catalysis, Tarragona, Spain, 1996
35. On the interaction of a CO molecule with an electron-deficient Pt atom in mordenite: a density functional model cluster study. – Second Conference on “Modern Trends in Chemical Kinetics and Catalysis”, Novosibirsk, Russia, 1995

34. Clustermodellrechnungen zur Adsorption von NH auf einer Ru(001)-Oberfläche. – 95. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Bremen, Germany, 1995

33. Non-classical structures of adsorption complexes with NO and CO on metals and oxide materials. – Workshop on "Orientation in Molecule-Surface Interactions", Volendam, Holland, 1994

32. Density functional and vibrational spectroscopy study of N_2 and CO probes adsorbed at Lewis and Brönsted acid sites in aluminosilicates. – The satellite meeting of VIII International congress on quantum chemistry on "Quantum chemical aspects of heterogeneous catalysis", Berlin, Germany, 1994

31. Non-classical structures of adsorption complexes with CO and NO on metals and oxide materials. – 93. Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie, Berlin, Germany, 1994

30. Vibrational characteristics of adsorption complexes on the surface of ionic crystals: A density functional study. (presented by N. Rösch) – WE-Heraeus-Seminar "Adsorption on ordered surfaces of ionic solids and thin films", Bad Honnef, Germany, 1993

29. Density functional studies of adsorption at metal oxide surfaces. – 13th European conference on surface science. Warwick, United Kingdom, 1993

28. Bonding and vibrations of CO molecule adsorbed on surface of ionic crystals. – XXI European congress on molecular spectroscopy. Vienna, Austria, 1992

27. Cluster models of chemisorption: Applications and limitations. – 28th Symposium on Theoretical Chemistry, Brixen, Italy, 1992.

26. Bonding and vibrations of weakly adsorbed diatomic molecules on metal and insulating surfaces: density functional model cluster studies. –XII International vacuum congress / VIII International conference on solid surface. The Hague, Netherlands, 1992.

25. Cluster LCGTO-LDF models of adsorption on ionic crystals: bonding and vibrations of CO molecule on MgO surface. – 4th International symposium "Theoretical approach to catalysis at interfaces". Cracow, Poland, 1992

24. Adsorption of CO on MgO surface: analysis of LCGTO-LDA cluster models. – 91. Hauptversammlung der Deutschen Bunsen-Gesellschaft fur Physikalische Chemie. Vienna, Austria, 1992

23. Electronic interactions and geometrical structure of adsorption systems. – Summary session of SFB 338, University of Munich, Germany, 1992

22. Quantum chemistry and spectroscopy of highly excited states of coordination compounds. – 23rd International conference on coordination chemistry. Gera, GDR, 1990

21. High-T_c superconductors of the La_2CuO_4 type: characteristic features of electronic properties of surface. - 3rd International symposium on elementary processes and chemical reactivity. Liblice, Czechoslovakia, 1989

20. Resonant X-ray emission in the spectra of d-metal coordination compounds. - XXVI Colloquium Spectroscopicum Internationale. Sofia, Bulgaria, 1989

19. Cluster modelling of electronic properties of La_2CuO_4-based materials: bulk and surface. - School on actual problems of physics and chemistry of rare-earth metal-based chemical compounds. Krasnoyarsk, USSR, 1989

18. X-ray resonant emission in spectra of transition and rare-earth metal complexes. - 15th All-Union conference on X-ray and electron spectroscopy. Leningrad, USSR, 1988

17. Nonempirical MO LCAO theory of $K\beta_5$ spectra of 3d-metal coordination compounds. – 15th All-Union conference on X-ray and electron spectroscopy. Leningrad, USSR, 1988
16. X-ray and photoelectron spectra and electronic structure of platinum metal hexahalogenide complexes. - 10th All-Union school-seminar “X-ray and electron spectra and chemical bonding”. Odessa, USSR, 1987
15. Quantum chemical ans X-ray spectral investigation of electronic structure of the iron subgroup metallocenes. - 9th All-Union conference “Physical and mathematical methods in coordination chemistry”. Novosibirsk, USSR, 1987
14. X-ray and X-ray photoelectron spectra and electronic structure of platinum metal hexahalogenide complexes. - 9th All-Union conference “Physical and mathematical methods in coordination chemistry”. Novosibirsk, USSR, 1987
13. Electronic structure of ferrocene, ruthenocene and osmocene: the data of the Xα SW calculations and X-ray spectroscopy. - 4th All-Union conference “Spectroscopy of coordination compounds”. Krasnodar, USSR, 1986
12. Spectra and electronic structure of hexahalogenide complexes of VIII group metals as calculated by cluster SCF Xα SW method. - 2nd All-Union conference “Quantum chemistry and spectroscopy of solids”. Sverdlovsk, USSR, 1986
11. Electronic structure and X-ray spectral characteristics of mononuclear carbonyl complexes as calculated by SCF Xα SW method. - 9th All-Union conference on quantum chemistry. Ivanovo, USSR, 1985
10. Resonant emission in the X-ray emission spectra. - All-Union conference “Quantum chemistry and spectroscopy of solids”. Sverdlovsk, USSR, 1984
9. Estimation of the bond strength of CO molecules interacting with surfaces by SCF Xα SW method. - 5th All-Union symposium on quantum theory of adsorption and catalysis. Moscow, USSR, 1984
8. A study of highly excited states of symmetrical metal complexes by the SCF Xα SW method. - International conference on X-ray and inner-shell processes in atoms, molecules and solids. Leipzig, GDR, 1984
7. Investigation of electronic structure of 3*d*, 4*d* and 5*d* metal complexes by the methods of X-ray and photoelectron spectroscopy and X scattered wave. - VIII All-Union school-seminar “X-ray and electron spectra and chemical bonding”. Vladivostok, USSR, 1983
6. SCF Xα SW and X-ray spectral investigation of electronic structure of d-metal coordination compounds. - VIII All-Union conference “Physical and mathematical methods in coordination chemistry”. Kishinev, USSR, 1983
5. *Ab initio* investigation of resonances in X-ray absorption spectra of molecules SCO, CS_2 and SO_2. – Conference “X-ray and X-ray photoelectron spectra and electronic structure of metals, alloys and chemical compounds”. Izhevsk, USSR, 1979
4. Many-particle effects in X-ray spectra of molecules. Limitations of the orbital model. - Conference “X-ray and X-ray photoelectron spectra and electronic structure of metals, alloys and chemical compounds”. Izhevsk, USSR, 1979
3. *Ab initio* calculations of X-ray transitions in molecules. - XII All-Union conference on X-ray spectroscopy. Leningrad, USSR, 1978
2. Near-edge fine structure of X-ray absorption spectra of molecules. Method of quasistationary states. - XII All-Union conference on X-ray spectroscopy. Leningrad, USSR, 1978
1. Theoretical investigation of highly excited states of molecules. - VII All-Union conference on quantum chemistry. Novosibirsk, USSR, 1978

Other participation in national and international conferences

Chairing scientific sessions

46. 1st morning session, December 1, 2025 - 6th Int. Meeting on Nanoalloys, Barcelona, Spain
45. 1st afternoon session, November 21, 2024 - International workshop "Twins in catalysis: Merging theory and experiment", Barcelona, Spain
44. Morning session, October 31, 2024 - IQTC meeting 2024, Faculty of Chemistry, Universitat de Barcelona, Barcelona, Spain
43. Afternoon session, April 3, 2022 - Cluster-Surface Interaction workshop (CSI2022), Santa Margherita Ligure, Italy
42. On-line session 6 "Physical-chemical fundamentals of catalysis / Industrial implementation of catalytic processes", October 9, 2020 - VI International School-Conference for Young Scientists "Catalysis: from Science to Industry", Tomsk, Russia
41. Session "Basic concepts, theory and modeling in catalysis - I", October 8, 2019 - XI International Conference "Mechanisms of Catalytic Reactions", Sochi, Russia
40. Afternoon session, August 21, 2019 - Symposium "Nano-alloys: Theory, Synthesis & Characterization", XXVIII International Materials Research Congress, Cancún, Mexico
39. Session "Nanoparticles on surfaces", December 3, 2018 - CECAM Workshop "Modeling metal-based nanoparticles: environment and dynamical effects", Grenoble, France
38. 2nd International Symposium on Single-Atom Catalysis, Beijing, China, June 17, 2018
37. III Russian Congress on Catalysis "Roskataliz-2017", Nizhny Novgorod, Russia, May 24, 2017
36. Joint 4th Energy Materials Workshop of the Thomas Young Centre and TOUCAN International Conference "Shaping Nanocatalysts", London, UK, December 14-16, 2016
35. X International Conference "Mechanisms of Catalytic Reactions", session "First-principles approach, theory and simulation in catalysis", Svetlogorsk, Russia, October 3, 2016
34. International Symposium on Single-Atom Catalysis (Satellite Meeting of the 16th International Congress on Catalysis), Dalian, P.R. China, June 30 - July 2, 2016
33. 16th International Conference on Theoretical Aspects of Catalysis (ICTAC-16), Zakopane, Poland, June 19-23, 2016
32. WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Poznan, Poland, November 26-27, 2015
31. 4th International Workshop "New Trends in Computational Chemistry for Industry Applications", Barcelona, Spain, October 1-2, 2015
30. International CECAM Workshop "Modeling Metal-based Nanoparticles: Toward Realistic Environments", CECAM-FR-GSO, CEMES, Toulouse, France, June 30, 2015
29. International Workshop "Low-precious-metal-content catalysts for PEM fuel cells", Dijon, France, June 8-11, 2015
28. WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions", Charles University in Prague, Czech Republic, May 8-9, 2014
27. Meeting of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Santa Margherita de Ligure, Italy, April 6-9, 2014
26. China-Europe International Workshop on Alloy Nanoparticles, Beijing, P. R. China, November 18-21, 2013

25. Symposium on Experimental and Theoretical Studies of Ceria, Barcelona Knowledge Campus of International Excellence and Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, October 7, 2013
24. 3rd Symposium of the Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, November 23, 2012
23. Joint Working Group Meetings of the COST Action MP0903 "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Antalya, Turkey, November 19-21, 2012
22. IX International Conference "Mechanisms of Catalytic Reactions" (MCR-2012), St. Petersburg, Russia, October 22-25, 2012
21. CECAM (ZCAM) Workshop "Modelling realistic inorganic nanostructures; bridging the gap between theory and experiment", Zaragoza, Spain, September 5-7, 2012
20. Session "Advances in Computational Catalysis" on July 4th of the 15th International Congress on Catalysis, Munich, Germany, July 1-6, 2012
19. 2nd International Symposium on Intermetallic Compounds in Methanol Steam Reforming, Munich, Germany, June 27-28, 2012
18. Working Groups Meeting of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications", Limerick, Ireland, October 12-14, 2011
17. Satellite Meeting on "Theoretical Modelling of Materials" to the WATOC-2011 Congress, Barcelona, Spain, July 13-15, 2011
16. European CECAM Workshop "Understanding ceria based materials in catalysis - a challenge for theory and experiment", Zaragoza, Spain, June 20-23, 2011
15. International Workshop "New Trends in Computational Chemistry for Industry Applications", University of Barcelona, Barcelona, Spain, May 26-27, 2011
14. Joint Working Group Meetings of the European COST Action MP0903 "Nanoalloys", Barcelona, Spain, April 14-16, 2011
13. Scientific Kick-off Meeting of the European COST MP0903 Action "Nanoalloys", Genova, Italy, October 18-20, 2010
12. 4th Humboldt Conference on Computational Chemistry, Varna, Bulgaria, July 12-15, 2010
11. Primeres Jornades Doctorals del Departament de Química Fisica (First Conference of Doctoral Students of the Physical Chemistry Department), Universitat de Barcelona, Barcelona, Spain, February 5, 2010
10. European COST D41 Action "Inorganic Oxides: Surfaces and Interfaces", Workshop of the Working Group 1 on "Oxide Nanostructures", Erlangen, Germany, April 16-18, 2009
9. International Workshop on Computational Catalysis, Catalysis Research Centre, TU München, Garching, Germany, January 7-9, 2009
8. Symposium "Density-Functional Methods and their Applications", Garching, Germany, November 7, 2008
7. 12th International Conference on Theoretical Aspects of Catalysis, Varna, Bulgaria, June 25-29, 2008
6. International Workshop "Towards Reality in Nanoscale Materials", Levi, Finland, December 10-12, 2007
5. European COST D41 Action "Inorganic Oxides: Surfaces and Interfaces", Annual Meeting, Berlin, Germany, October 21-23, 2007

4. European COST D41 Action “Inorganic Oxides: Surfaces and Interfaces”, Workshop on “Oxide Nanostructures”, Barcelona, Spain, May 10-12, 2007
3. International Workshop “Supported Metal Clusters”, TU München, Munich, Germany, July 6-7, 2006
2. WE-Heraeus-Seminar “Energetics of Interfaces between Organic Molecules and Conductors”, Bad Honnef / Bonn, Germany, March 20-22, 2003
1. EURESCO European Conference on Fundamental Aspects of Surface Science “Structure and Reactivity of Oxide Surfaces”, Acquafredda di Maratea, Italy, June 1-6, 2002

Organization of conferences

30. Co-organizer of the 6th International Meeting on Nanoalloys (IMN 2025), Barcelona, Spain, on December 1- 4, 2025
29. Organizer of the International Symposium “Density Functional Theory, Sorption and Catalysis”, Garching b. München, Germany, September 8, 2023
28. Scientific Committee Member of the 6th Intern. School on Catalysis for Young Scientists “Catalyst Design: From Molecular to Industrial Level”, Novosibirsk, Russia, May 16-19, 2021
27. Co-organizer of the International Symposium on the DFT Modelling of Materials Relevant for Water Splitting (virtual), Barcelona, Spain, December 11, 2020
26. Member of the Scientific Committee of the XI International Conference on Mechanisms of Catalytic Reactions, Sochi, Russia, October 7-11, 2019
25. Co-organizer of the Symposium “Nano-alloys: Theory, Synthesis & Characterization”, XXVIII International Materials Research Congress, Cancún, Mexico, August 18-23, 2019
24. Co-organizer of the Symposium “Nano-alloys: Theory, Synthesis & Characterization”, XXVII International Materials Research Congress, Cancún, Mexico, August 19-24, 2018
23. Member of the International Scientific Committee of the 3rd International Conference “Fundamentals and applications of cerium dioxide in catalysis”, Barcelona, Spain, June 25-27, 2018
22. Member of the Scientific Committee of the 5th International School-Conference on Catalysis for Young Scientists “Catalyst Design: From Molecular to Industrial Level”, Moscow, Russia, May 20-23, 2018
21. Member of the Scientific Committee of the X International Conference on Mechanisms of Catalytic Reactions and discussion leader of the School-Symposium “Quantum-mechanical modelling of catalytic processes”, Svetlogorsk, Russia, October 3-7, 2016
20. Organizer and co-chairman of the Discussion Symposium “DFT calculation in catalytic studies” within the XII European Congress on Catalysis (EuropaCat) “Catalysis: Balancing the use of fossil and renewable resources”, Kazan, Russia, August 30 - September 4, 2015
19. Organizer of the General Assembly and Management Committee meetings of the FP7 project “Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology”, Barcelona, Spain, December 11-12, 2014 (16 participants from 6 countries)
18. Co-organizer of the Symposium “Frontiers in surface and materials science: theory and practice”, Barcelona, Spain, November 14, 2014. (140 participants from 20 countries)
17. Chairman and local organizer of the 3rd General Meeting of the COST Action CM1104 “Reducible oxide chemistry, structure and functions”, Barcelona, Spain, November 12-14, 2014. (120 participants from 22 countries)

16. Organizer of the Symposium “Clusters, nanoparticles and nanostructures in catalysis and beyond”, Computational Material Science Laboratory, IQTCUB, Barcelona, June 27, 2014 (18 participants from 3 countries)
15. Co-organizer of the 5th Symposium of the Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, May 30, 2014
14. Organizer of the General Assembly and Management Committee meetings of the FP7 project “Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology”, Barcelona, Spain, January 31, 2014 (18 participants from 5 countries)
13. Co-organizer of the 4th Symposium of the Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, June 21, 2013 (65 participants)
12. Co-organizer of the 3rd Symposium of the Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, November 23, 2012 (70 participants)
11. Co-organizer of the 2nd International Symposium on Intermetallic Compounds in Methanol Steam Reforming, Munich, Germany, June 27-28, 2012 (45 participants from 12 countries) http://www.symposium.methanol-to-hydrogen.eu/index.php
10. Co-organizer of the Danish-Spanish Workshop on Modelling of Inorganic Materials and Surfaces, Barcelona, Spain, October 20, 2011 (25 participants)
9. Chairman of the local Organizing Committee of a Satellite Meeting for the WATOC 2011 Congress “Theoretical modelling of materials”, Barcelona, Spain, July 13-15, 2011 (~100 participants from ~20 countries)
8. Co-chairman of the CECAM Workshop “Understanding ceria based materials in catalysis - a challenge for theory and experiment”, Zaragoza, Spain, June 20-23, 2011 (63 participants from 17 countries)
7. Organizer of the 2nd Symposium of the Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, April 29, 2011
6. Chairman of the Annual Meeting of the European COST Action MP0903 “Nanoalloys”, Barcelona, Spain, April 14-16, 2011 (92 participants from 23 countries)
5. Organizer of the 1st Symposium of the Institute of Computational and Theoretical Chemistry of the University of Barcelona (IQTCUB), Barcelona, Spain, May 14, 2010
4. Organizer of the Symposium “Density-Functional Methods and their Applications” (in honour of Prof. N. Rösch), Garching, Germany, November 7, 2008 (~50 participants)
3. Organizer of the Annual Meeting of the European COST-D41 Action “Inorganic Oxides: Surfaces and Interfaces”, Barcelona, Spain, October 16-18, 2008 (64 participants from 13 countries)
2. Member of the International Scientific Committee of the International Conference “Material Informatics and DFT”, Oran, Algeria, October 11-13, 2008
1. Co-chairman of the Workshop “Oxide Nanostructures” of the European COST D41 Action “Inorganic Oxides: Surfaces and Interfaces”, Barcelona, Spain, May 10-12, 2007 (30 participants from 6 countries)

Recent PhD and Master Theses (selection)

Supervision of PhD theses (2014 - present)

Riccardo Farris, *Development and application of advanced computational methods for predicting the structure and properties of nanoparticles*, excellent - cum laude, Universitat de Barcelona, Departament de Ciència de Materials i Química Física. November 21, 2025. Co-supervision with Dr. Albert Bruix.

Pablo Castro Latorre, *Exploring the complexity of nanostructured catalysts using computational modelling methods*, excellent, Universitat de Barcelona, Departament de Ciència de Materials i Química Física. September 16, 2025. Co-supervision with Dr. Albert Bruix.

Jon Eunan Quinlivan Domínguez, *Application and development of machine-learning assisted global optimization algorithms for heterogeneous catalysis*, excellent, Universitat de Barcelona, Departament de Ciència de Materials i Química Física. April 25, 2025. Co-supervision with Dr. Albert Bruix.

Lorena Vega Domínguez, *Advanced modelling of metallic nanomaterials for catalysis*, excellent - cum laude, Universitat de Barcelona, Departament de Ciència de Materials i Química Física, December 21, 2021. Co-supervision with Dr. Francesc Viñes.

Alberto Figueroba Sánchez, *Density functional modelling of materials for fuel cell catalysts with reduced content of critical components*, excellent, Universitat de Barcelona, Departament de Ciència de Materials i Química Física, July 14, 2017.

Sergey M. Kozlov, *A study of nanostructuring effects on model heterogeneous catalysts*, excellent - cum laude, Universitat de Barcelona, Depart. de Química Física, January 16, 2015.

Albert Bruix Fusté, *Computational modeling of heterogeneous catalysts based on platinum and cerium oxide*, excellent - cum laude, Universitat de Barcelona, Departament de Química Física, February 17, 2014. Co-supervised with Prof. Francesc Illas.

Supervision of Master theses (2009 - present)

Elena Zerbato, *Effect of oxygen adsorption on optical properties of Ag nanoparticles*, Università di Trieste (Italy), Dipartimento di Scienze Chimiche e Farmaceutiche, July 22, 2022. Co-supervision with Prof. Mauro Stener.

Nicola Danielis, *Silver and gold nanoalloys: interplay between chemical ordering and optical properties*, Università di Trieste (Italy), Dipartimento di Scienze Chimiche e Farmaceutiche, July 22, 2020. Co-supervision with Prof. Mauro Stener.

Sofia Olobardi, *Chemical ordering in Ag-Pt nanoalloys: structures and spectra*, Università di Trieste (Italy), Dipartimento di Scienze Chimiche e Farmaceutiche, July 11, 2019. Co-supervision with Prof. Mauro Stener.

Jordi Toda Calderón, *Theoretical study of the interaction of Pt atoms with ceria nanoparticles*, Universitat de Barcelona, Departament de Química Física, September 9, 2011.

Albert Bruix Fusté, *First-principles study of platinum atoms / ceria(111) surface interactions*, Universitat de Barcelona, Departament de Química Física, September 9, 2009.

Member of PhD thesis Defence Committees (2015 - present)

1. Committee member (examiner) – PhD thesis defence of Laura Hargreaves
   Title "Computational Modelling of Molecular Adsorption on Oxide Surfaces at Different Coverages", University College London (UK); June 12, 2024
2. Committee member substitute – PhD thesis defence of Marc Figueras Valls
   Title: "Nanostructured transition metal carbides as potential catalysts for greenhouse gases conversion", Universitat de Barcelona (Spain); December 14, 2021
3. Committee member (president) – PhD thesis defence of Antoni Macià Escatllar
   Title "Computational Modelling of TiO_2 and Mg-silicate nanoclusters and nanoparticles - Crystallinity and astrophysical implications"
   Universitat de Barcelona (Spain); September 4, 2020
4. Committee member substitute – PhD thesis defence of Hèctor Prats Garcia
   Title: "Monte Carlo based methods applied to heterogeneous catalysis and gas separation"
   Universitat de Barcelona (Spain); March 25, 2019
5. Committee member – PhD thesis defence of Andi Cuko
   Title "Modelling nano-oxide materials with technological and environmental relevance: Silica, Titania and Titanosilicates"
   Sorbonne Universitè, Paris (France) & Universitat de Barcelona (Spain); September 24, 2018
6. Committee member – PhD thesis defence of Josep Oriol Lamiel Garcia
   Title "Desenvolupament de models per nanopartícules de TiO_2 i ZnO en fotocatálisis"
   Universitat de Barcelona (Spain); September 27, 2017
7. Committee member – PhD thesis defence of Javier Tirso López Auséns
   Title "From Quantum Mechanics to Catalysis: Studies on the oxidation of alkanes by gold and metal oxides"
   Universitat Politècnica de València (Spain); December 12, 2016
8. Committee member – PhD thesis defence of Samuel Rowan Bradley
   Title "Computational modelling of oxygen defects and interfaces in monoclinic HfO_2"
   University College London (UK); October 29, 2015