

Sergey Kozlov

Resume

Assistant Professor at the Department of Chemical and Biomolecular Engineering, National University of Singapore

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ORCID: [0000-0002-7765-4649](https://orcid.org/0000-0002-7765-4649)

Date of birth: 02 June 1986



Appointments

Jun 2019 – now	Assistant Professor	National University of Singapore
Jan 2016 – Jun 2019	Postdoctoral Fellow	King Abdullah University of Science and Technology
Nov 2014 – Jan 2016	Postdoctoral Fellow	Universitat de Barcelona
Dec 2010 – Nov 2014	PhD Researcher	Universitat de Barcelona
Jan 2010 – Nov 2010	Research Assistant	Universität Erlangen-Nürnberg
Jun 2006 – May 2008	Laboratory Assistant	Boreskov Institute of Catalysis

Education

2015	PhD in Chemistry	University of Barcelona
2009	MSc in Physics	Novosibirsk State University
2007	BSc in Physics	Novosibirsk State University

Research Track

Co-author of 72 papers (including **3 Nature Materials**, **1 Nature Catalysis**) and 1 book chapter
5800+ citations (h-index = 43) with 4 of my articles considered highly cited
1 plenary, 1 keynote and 13 invited talks among 62 oral presentations at scientific conferences

Major Research Projects (5.8M € including smaller grants)

- 2024-2027 **(Leading a team of 2 PIs)** “*Rational Design and Manufacturing of Photothermal Catalytic Membranes for Water-Energy Nexus*” In this Individual Research Grant by A*Star, we achieved the computational design of two new catalysts for CO oxidation and electrochemical hydrogen evolution in the form of metal-supported oxide films.
- 2022-2025 **(Leading a team of 6 PIs)** “*Nanostructured Catalysts for Direct CO₂ Hydrogenation to Higher Alcohols and Fuels*” In this grant by the Low-Carbon Energy Research Funding Initiative, we developed new catalysts for commercially feasible production of sustainable aviation fuels (SAFs) using CO₂ and blue H₂ as feedstock.
- 2021-2026 **(Sole PI)** “*Rational Design of Catalysts Enhanced by Nanoscale Metal-Oxide Interactions*” In this fellowship by the National Research Foundation of Singapore for the project, we achieved computational design of nanocomposite catalysts for selective methane chlorination and high-entropy alloys for NH₃ synthesis.

Industrial Collaborations

TotalEnergies (France), SABIC (Saudi Arabia), NuStar Technologies (Singapore)

Publication Track

72 articles and 1 book chapter, 5800+ citations, h-index 43

[†] co-first author; * corresponding author

Knebel, Bavykina, Datta, Sundermann, Garzon-Tovar, Lebedev, Durini, Ahmad, [Kozlov](#), Shterk, Karunakaran, Carja, Simic, Weilert, Klüpel, Giese, Cavallo, Rueping, Eddaoudi, Caro, Gascon, *Solution processable metal–organic frameworks for mixed matrix membranes using porous liquids*, **Nat. Mater.** 2020, 19, 1346

Suchorski,[†] [Kozlov](#),[†] Bespalov, Datler, Vogel, Budinska, Neyman, Rupprechter, *The role of metal-oxide interfaces for long range metal particle activation during CO oxidation*, **Nat. Mater.** 2018, 17, 519

Lykhach,[†] [Kozlov](#),[†] Skála, Tovt, Stetsovych, Tsud, Dvořák, Johánek, Neitzel, Mysliveček, Fabris, Matolín, Neyman, Libuda, *Counting electrons on supported nanoparticles*, **Nat. Mater.** (**highly cited article**) 2016, 15, 284

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Zhang, Wang, Cao, [Kozlov](#), García de Arquer, Dinh, Li, Wang, Zheng, Zhang, Wen, Voznyy, Comin, De Luna, Regier, Bi, Alp, Pao, Zheng, Hu, Ji, Li, Zhang, Cavallo, Peng, Sargent, *High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics*, **Nat. Catal.** (**highly cited article**) 2020, 3, 985

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Wang, Cao, Zheng, Zhang, [Kozlov](#), Chen, Zou, Kong, Wen, Liu, Zhou, Dinh, Zheng, Peng, Zhao, Cavallo, Zhang, Sargent, *Hydration-Effect-Promoting Ni–Fe Oxyhydroxide Catalysts for Neutral Water Oxidation*, **Adv. Mater.** 2020, 32, 1906806

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Gao, Tianxi Zhang, Ng, Lu, Tian, Ong, [Kozlov](#), Ho, *Polymeric Layered Films for TiO₂-Au/CuS Tandem Photothermal Catalytic H₂ Production in Harsh Seawater and Waste Plastic Media*, **Adv. Ener. Mat.**, 2025, DOI: 10.1002/aenm.202404198

Zhong, Cao, Yang, [Kozlov](#), Huang, Tung, Cavallo, Li, Han, *Electrochemical Conversion of CO₂ to 2-Bromoethanol in a Membraneless Cell*, **ACS Energy Letters** 2019, 4, 600

Sheng, Polynski, Eswaran, Zhang, Lim, Zhang, Jiang, Liu,* [Kozlov,*](#) *A review of mechanistic insights into CO₂ reduction to higher alcohols for rational catalyst design*, **Appl. Cat. B** 2024, 343, 123550

Zhou, Ma, Kosari, Lim, [Kozlov,*](#) Zeng,* *Highly Active Single-layer 2H-MoS₂ for CO₂ Hydrogenation to Methanol*, **Appl. Cat. B**. 2024, 349, 123870

Lee, Anjum, Araújo, Mondelli, He, Furukawa, Pérez-Ramírez,* [Kozlov,*](#) Yan,* *Atomic Pd-promoted ZnZrO_x solid solution catalyst for CO₂ hydrogenation to methanol*, **Appl. Cat. B** 2022, 304, 120994
(highly cited article)

AlSabban, Falivene, [Kozlov](#), Aguilar-Tapia, Ould-Chikh, Hazemann, Cavallo, Basset, Takanabe, *In-operando elucidation of bimetallic CoNi nanoparticles during high-temperature CH₄/CO₂ reaction*, **Appl. Cat. B** 2017, 213, 177

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Chepkasov, Baidyshev, Golubnichiy, Zamulin, Kvashnin, [Kozlov,*](#) *Cu-Au Nanoparticles Produced by the Aggregation of Gas-Phase Metal Atoms for CO Oxidation*, **Aggregate**, 2022, e273

Nilius, [Kozlov](#), Jerratsch, Baron, Shao, Viñes, Shaikhutdinov, Neyman, Freund, *Formation of one-dimensional electronic states along the step edges of CeO₂ (111)*, **ACS Nano** 2012, 6, 1126

Aleksandrov, [Kozlov](#), Schauermaun, Vayssilov, Neyman, *How absorbed hydrogen affects catalytic activity of transition metals*, **Angew. Chem. Int. Ed.** 2014, 53, 13371

Zhou, Ma, Anjum, Kosari, Xi, [Kozlov](#), Zeng, *Strained few-layer MoS₂ with atomic copper and selectively exposed in-plane sulfur vacancies for CO₂ hydrogenation to methanol*, **Nat. Commun.** 2023, 14, 5872

Chen, Aliasgar, Zamudio, Zhang, Zhao, Lian, Wen, Yang, Sun, [Kozlov,*](#) Chen, Wang,* *Diversity of platinum-sites at platinum/fullerene interface accelerates alkaline hydrogen evolution*, **Nat. Commun.** 2023, 14, 1711 **(highly cited article)**

Lee, Mendes, Jeon, Song, Dickieson, Anjum, Chen, Yang, Yang, Choi, [Kozlov,*](#) Yan,* *Engineering nanoscale H supply chain to accelerate methanol synthesis on ZnZrO_x*, **Nat. Commun.** 2023, 14, 819

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Das, Anjum, Lim, He, Hoffman, Bare, [Kozlov](#), Gates, Kawi, *Genesis of Active Pt/CeO₂ Catalyst for Dry Reforming of Methane by Reduction and Aggregation of Isolated Platinum Atoms into Clusters*, **Small**, 2023, 2207272

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[Kozlov](#),* Neyman,* *Effects of electron transfer in model catalysts composed of Pt nanoparticles on CeO₂(1 1 1) surface*, **J. Catal.** 2016, 344, 507

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Janthon, Luo, [Kozlov](#), Viñes, Limtrakul, Truhlar, Illas, *Bulk properties of transition metals: a challenge for the design of universal density functionals*, **J. Chem. Theory Comput. (ACS Editors' Choice)** 2014, 10, 383

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[Kozlov](#), Cabeza, Neyman, *Bonding and vibrations of CH_xO and CH_x species (x = 1–3) on a palladium nanoparticle representing model catalysts*, **Chem. Phys. Lett.** 2011, 506, 92

Book Chapter:

[Kozlov](#), Aleksandrov, Moskaleva, Bäumer, Neyman. Chapter 7.18 - *From static to reacting systems on transition-metal surfaces*. In: **Comprehensive Inorganic Chemistry (2nd edition)**, Eds. J. Reedijk, K. Poeppelmeier, Vol. 7: Surface Inorganic Chemistry and Heterogeneous Catalysis, Eds. R. Schlögl, J. W. Niemantsverdriet, Elsevier, Oxford, 2013, p. 47

Funding Track

As Lead PI (2832k € total):

2024-2027 Individual Research Grant by Agency for Science, Technology and Research
946k S\$ (A*STAR) “*Rational Design and Manufacturing of Photothermal Catalytic Membranes for Water-Energy Nexus*”
(~673 k€) Co-I: Ghim Wei Ho (NUS)

2022-2025 Low-Carbon Energy Research Funding Initiative grant by Agency for
3034k S\$ Science, Technology and Research (A*STAR) “*Nanostructured Catalysts for Direct CO₂ Hydrogenation to Higher Alcohols and Fuels*”.
(~2159 k€) Team PI: Paul Wen Liu (NTU); Lili Zhang (A*Star ISCE²)
Co-I: He Qian (NUS) and Jiang Jianwen (NUS), Amol Hegne (A*Star ISCE²)
Collaborators: Ifterkhar A. Karimi (NUS) and Shamsuzzaman Farooq (NUS);
Industry Collaborator: NuStar Technologies (Singapore)

As a Sole PI (2492k € total):

2021-2026 Fellowship by the National Research Foundation of Singapore for project
2756k S\$ “*Rational Design of Catalysts Enhanced by Nanoscale Metal-Oxide Interactions*”
(~1961k €)

2019-2023 Start-up grant “*Electrochemical CO₂ reduction on nanostructured Cu catalysts*”
600k S\$ from the National University of Singapore composed of 250k S\$ in research funding
(~430 k€) and 450k S\$ support in the form of research scholarships for 2 PhD students.

2020-2022 “*Simulations of Zn-Zr mixed oxide catalysts for methanol production*” grant from
142k S\$ Green Energy Flagship Program of the National University of Singapore
(~101 k€)

As co-PI (415k € total):

2024-2027 CREATE program by National Research Foundation of Singapore “*Development of*
583k S\$ *Advanced Catalysts for Electrochemical Carbon Abatement*” (total budget 5300k S\$)
(~415k €) Lead PI: CHEN Wei (NUS)
Co-PI: LU Jiong (NUS), Yanwei LUM (NUS), Ming ZHAO (NUS), Zhichuan Jason XU (NTU), Adrian FISCHER (Cambridge), Yugen ZHANG (A*Star ISCE²)

Scholarships (60k € total):

2010 FPU (Formation of University Professors) scholarship AP2009-3379 “*Particularities*
60k € *of nanoparticle models in catalysis compared to slab models: Studies of surface reactivity based on density functional theory*” from the Spanish Ministry of Education, Culture and Sport to support PhD studies at the University of Barcelona

CPU time procurement (86 M CPU×h, equivalent to 477k €)

2020-2024 63 M CPU×h (378k S\$ ~267k €)	Grants 1621 “ <i>Nanostructured catalysts for methanol synthesis</i> ”, 1915 “ <i>CO₂ reduction over nanostructured Cu-based catalysts</i> ”, 2183 “ <i>Oxygen reduction reaction on Pt and Pd-based nanoalloy catalysts</i> ”, 2347 “ <i>Simulations of metal-oxide nanocomposites</i> ”, 3808 “ <i>Rational Design of Trimetallic Alloy Nanoparticle Catalysts for CO₂ hydrogenation into C₂+ alcohols</i> ”, 4217 “ <i>Development of Advanced Catalysts for Electrochemical Carbon Abatement</i> ”, 4220 “ <i>Rational Design and Manufacturing of Photothermal Catalytic Membranes for Water-Energy Nexus</i> ” on National Supercomputing Center, Singapore
2016-2018 22M CPU×h (~204k €)	Grants k1133 “ <i>Computational identification of transition metals strongly affected by nanostructuring</i> ”, k1214 “ <i>Optical and catalytic properties of alloy nanoparticles</i> ”, k1322 “ <i>In-Cu catalysts for electrochemical CO₂ reduction</i> ” and k1397 “ <i>NiMo catalysts for hydrogen evolution reaction</i> ” on Shaheen II supercomputer, Saudi Arabia
2015-2016 0.6M CPU×h (~6k €)	Grant QCM-2015-3-0031 “ <i>Ternary alloy particles for improved oxygen reduction reaction catalysts</i> ” on Memento machine of Spanish Supercomputing Network (RES)

Conference Track

Besides 1 plenary, 1 keynote, and 12 invited talks outlined below, I also delivered 12 invited seminars at various universities and 47 oral presentations at various congresses. In turn, my group members at NUS delivered 8 oral and 23 presentations at various conferences.

Conference organization:

2. Computational Catalysis & AI section of the 10th Asia-Pacific Congress on Catalysis (APCAT 10), Singapore, 4-7 August 2025
1. Computational Catalysis section of the 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP 2024), Qingdao, China, 13-18 October 2024

Plenary and keynote lectures:

2. (keynote) S. M. Kozlov, “Chemical Properties of Metal-Oxide Interfaces in Heterogeneous Catalysts” at the 105th Chemical Society of Japan Annual Meeting, 26-29 March 2025, Suita, Japan
1. (plenary) S. M. Kozlov, “Increasing Activity of Heterogeneous Catalysts by Metal-

Oxide Interactions” at XII International Conference “Mechanism of Catalytic Reactions” (MCR-XII), Vladimir, Russia, 17-24 June 2024

Invited talks at Scientific Conferences:

13. S. M. Kozlov, “Increasing the range of nanoparticle-support interactions in catalysis” at 12th Singapore International Chemistry Conference (SICC-12), Singapore, 9-13 December 2024
12. S. M. Kozlov, “Role of Metal-Oxide Interfaces in Catalysis” at 11th Congress of the International Society for Theoretical Chemical Physics (ISTCP-2024) in Qingdao, China, 13-18 October 2024
11. S. M. Kozlov, “Oxide and sulfide-based catalysts for CO₂ reduction to methanol” at the 27th International Annual Symposium on Computational Science and Engineering (ANSCSE 27), Bangkok, Thailand, 30 July – 3 August 2024
10. S. M. Kozlov, “Nanocomposite catalysts for CO₂ reduction to methanol” at Fundamental Principles of Catalysis workshop 2023, Moscow, 27-28 November 2024
9. S. M. Kozlov, “Realistic Simulations of Nanocomposite Catalysts Based on Transition Metals” at the 10th conference of the Asia Pacific Association of Theoretical and Computational Chemistry (APATCC-10), Quy Nhon, Vietnam, 19-23 February 2023
8. S. M. Kozlov, A. Subramanian, “Simulations of alloy nanocrystallites for catalysis” at the XXX International Materials Research Congress, Cancun, Mexico, 14-19 August 2022
7. S. M. Kozlov, “Promoting catalytic activity by charge transfer between oxides and transition metal particles or dopants” at 1st International Conference on Energy Materials (ICEM) 2021, Kuala Lumpur, Malaysia, 5-8 November 2021
6. S. M. Kozlov, “Simulating nanocomposite catalysts at the atomic scale” at Singapore Catalysis Society's Annual General Meeting 2021, Singapore 25 October 2021
5. S. M. Kozlov, “Computational characterization of nanocomposite materials for catalysis” at Asia Pacific Society for Materials Research 2021 Annual Meeting, online, 20-23 August 2021
4. S. M. Kozlov, “Calculations of Nanostructured Materials” at IV International Symposium "Modern Materials Science" (MMS-2020), Moscow, Russia, 29 October 2019
3. S. M. Kozlov, “Realistic Modelling of Alloy Nanocrystallites with Hundreds of Atoms” at XXVII International Materials Research Congress (IMRC), Cancun, Mexico, 19-24 August 2018.

2. S. M. Kozlov, "Reactivity of Alloy and Supported Nanoparticles" at International Conference on Chemical Bonding, Kauai, USA, 13-17 July 2018
1. S. M. Kozlov, K. M. Neyman, "Nanostructured metal oxides and transition metal nanoparticles interacting with oxide surfaces from density-functional modeling" at CECAM workshop: Emergent structural and electronic phenomena at interfaces of nanoscale oxides, Lausanne, Switzerland, 8-10 April 2015

Chaired Sessions:

2. Chair morning session at the Computational Catalysis section of the 11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP 2024), Qingdao, China, 13-18 October 2024
1. Plenary session with Sir David MacMillan at Global Young Scientists Summit 2023, Singapore, 17-20 January 2023

Student Supervision

Graduated PhD students:

- 03.08.2020 – 19.11.2024 Yizhen Song "Computational studies of oxide catalysis promoted by transition metals" (degree awarded on 31.01.2025)
- 03.08.2020 – 06.11.2024 Arravind Subramanian "Computational modelling of alloy nanoparticles for catalysis" (degree awarded on 31.01.2025)

Current PhD students:

- | | |
|------------------|---|
| 02.08.2021 – now | Wenrui Ma "Simulations of Metal Oxides with Various Morphologies for Catalysis" |
| 02.08.2021 – now | Mohammed Aliasgar "Simulation and Atomistic Modelling of Supported Transition Metal Nanoparticles" |
| 10.01.2022 – now | Yifan Li "Machine learning techniques for materials discovery" (co-supervised with Dr. Shen Lei from the Department of Mechanical Engineering of NUS) |
| 01.08.2022 – now | Jie Zhao "Computational design of nanoparticle-support interfaces" |
| 01.08.2023 – now | Mingcan Chen "Development of Cu/ZnO catalysts for methanol synthesis" (co-supervised with Prof. Maoshuai Li from the University of Tianjin) |

Supervised Master students:

2024 – now	Bojun Xiao
2024	Nitilaksha Guduru
2021-2022	Hanbo Ding (now process engineer at ASM Pacific Technology)
2021	Savitha Srinivasan (now a PhD student at Chalmers University)

Supervised Undergraduate Students:

2025	Richard Lim Wei Boon, Dong Yihai, Feng Haoyuan, Goh Zhan Hong, team project supported by Undergraduate Research Experience (UREx) program
2025	Samuel Tan Qing Hui, Undergraduate Research Opportunities Program (UROP)
2025	Patrick Terrence Yu, Undergraduate Research Opportunities Program (UROP)
2023	Jiesheng Du, Undergraduate Research Opportunities Program
2022	Clemen Go Jia Gen, Undergraduate Research Opportunities Program (UROP)
2021	Eamon Malcolm Smith, academic exchange with Berkeley University through the SERIUS internship program
2020	Shawn Zi Ming Ng, Research Apprentice at NUS
2020	Wei Han Lin, Vacation internship program at NUS
2020	Emmanuel Alexander Junior Raj, Intern at NUS

Supervised Junior College Students:

02.12.2023-07.01.2024	Rachel Khor Wei Ning, Nanyang Junior College, Singapore
05.12.2022-23.12.2022	Jasper Leong Jun Quan, Nanyang Junior College, Singapore

Visiting Students:

23.08.2023 – 10.07.2024	Hao Chen	East China University of Science and Technology, China
25.10.2021 – 10.11.2021	Wang Tao	University of Tianjin, China
27.07.2022 – 04.09.2022	Chih-Heng Lee (Henry) 李知恆	National Tsing Hua University, Taiwan
13.01.2020 – 11.02.2020	Jerry 陳其伸	National Tsing Hua University, Taiwan

Teaching Track

2025 College Educator Award by NUS College of Design and Engineering
2023 College Teaching Excellence Award by NUS College of Design and Engineering

	Years	Class size	Contact hours per year	Student evaluation (faculty mean)	Difficulty evaluation (faculty mean)
Chemical Engineering Thermodynamics	2020-now	160-240	54-66	4 (4.1)	4.5 (3.6)
Advanced Reaction Engineering	2020-now	14-44	39	4.5 (4)	3.8 (3.6)

Teaching philosophy and innovations

I believe that universities should focus on creating supportive and engaging environments for *active* student learning. Therefore, I strive to maximize hands-on student learning while providing as much guidance and support as possible to the students in my classes.

In Chemical Engineering Thermodynamics, I use a flipped classroom approach with a significant (25%) blended learning component and facilitate intensive teacher-student dialogue during my lectures using Padlet.com. I also redesigned tutorial classes to focus on teamwork between students on provided pen-and-paper problems with me acting as a “guide on the side”.

In Advanced Reaction Engineering, I introduced hands-on atomistic simulations using the Atomic Simulations Environment package in Python or commercial Materials Studio software and updated the course narrative in line with current research approaches.

Service Track

10.2023 – now	Undergraduate Outreach Committee of the Department of Chemical and Biomolecular Engineering, National University of Singapore
09.2020 – 12.2023	Scholarship Committee of the Department of Chemical and Biomolecular Engineering, National University of Singapore
09.2020 – 12.2023	Coordinator of Academic Activities for Year 2 students in the Chemical Engineering undergraduate program, National University of Singapore
07.2019 – 09.2020	Social Committee of the Department of Chemical and Biomolecular Engineering, National University of Singapore

Reviewing activities

Reviewer of academic articles for Nature, Nature Catalysis, Nature Chemistry, Advanced Materials, Applied Catalysis B, Nature Communications, Nano Energy, Journal of American Chemical Society, ACS Nano, Angewandte Chemie, Small as well as 32 other journals.

Reviewer of grant proposals for the Center of Hydrogen Innovations of the National University of Singapore, OPUS-26 funding scheme by National Science Center Poland, and Tier 1 grants by the Ministry of Education of Singapore.

Examination committee members for 6 PhD students at the National University of Singapore, 1 PhD student at the University of Barcelona, 4 MSc students at the National University of Singapore, 1 MSc student at the National Tsing Hua University (Taiwan), and 1 MSc student at the Skolkovo University of Science and Technology (Russia).

External Awards

- 2023 Influential Researcher by Industrial & Engineering Chemistry Research Journal by American Chemical Society (IF = 3.8)
- 2023 Emerging Investigator Award from Journal of Materials Chemistry A by Royal Society of Chemistry (IF = 14.5)
- 2022 Emerging Investigator Award from Aggregate Journal by Wiley (IF = 13.9)