

Claudio Cazorla

Ramón y Cajal Research Fellow

Department of Physics, Universitat Politècnica de Catalunya

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Researcher IDs

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WOS ResearcherID: HKN-6203-2023

Education

2006 PhD in Computational Physics, Universitat Politècnica de Catalunya (Spain)

“Quantum Monte Carlo study of bosonic quantum solids at zero temperature”

Excellent Cum Laude, supervised by Prof. Jordi Boronat

2001 Bachelor in Physics, Universitat de Barcelona (Spain)

Research positions

2020-2025 Ramón y Cajal Research Fellow, Department of Physics, Universitat Politècnica de Catalunya (Spain)

2020-2024 Honorary Senior Lecturer, School of Materials Science and Engineering, UNSW Sydney (Australia)

2015-2020 Senior Lecturer, School of Materials Science and Engineering, UNSW Sydney (Australia)

2014-2019 ARC Future Research Fellow, School of Materials Science and Engineering, UNSW Sydney (Australia)

2011-2014 JAE-DOC Research Fellow, Institute of Materials Science of Barcelona (CSIC-ICMAB)

2010-2011 Postdoctoral Researcher, Institute of Materials Science of Barcelona (CSIC-ICMAB), Prof. M. Stengel's group

2006-2010 Postdoctoral Researcher, University College London (United Kingdom) Departments of Physics & Astronomy, Earth Sciences and Chemistry, Prof. M. J. Gillan's and Prof. D. Alfè's groups

Research and Funding achievements

- **>180 scientific publications** in peer review journals including *Nature*, *Nature Physics*, *Nature Communications*, *Science Advances*, *Reviews of Modern Physics*, *Physical Review Letters*, *Energy & Environmental Science*, *Advanced Materials*, *Advanced Energy Materials*, and *Advanced Functional Materials*
- **~ 6000 citations**, **h-index**: 45, **i10-index**: 132 (*Google Scholar*)
- **2.9 million €** in research funding as **Principal Investigator**
- **5.8 million €** in research funding as **Partner Investigator**

Fellowships/Awards

- 2020 Interdisciplinary Seed Funding **Award**, UNSW Sydney (Australia)
- 2019 Ramón y Cajal Research **Fellowship** (Spain)
- 2018 Postgraduate Research Supervision **Award**, UNSW Sydney (Australia)
- 2017 Visiting Research **Award**, Universitat de València (Spain)
- 2014 Australian Research Council Research **Fellowship** (Australia)
- 2011 JAE-DOC Research **Fellowship** (Spain)
- 2010 Translational Access HPC-Europa2 **Award** (Spain)
- 2009 Translational Access HPC-Europa2 **Award** (Spain)

Research funding as Principal Investigator

2022-2024 **Proyecto de Transición Ecológica y Digital 2021** (TED2021-130265B-C22): *Advanced theoretical and experimental characterization of low-dimensional chalcogenide materials and interfaces for their integration in solar cells*. Agencia Estatal de Investigación (Spain). Funding: **167,000 €**

2020-2025 **Ramón y Cajal Funding Grant** (RYC2018-024947-I): *Multicaloric materials for ambient solid-state cooling*. Agencia Estatal de Investigación (Spain). Funding: **315,000€**

2020-2023 **Discovery Projects 2021** (DP210100879): *Bioinspired flexible haptic memory materials for artificial sensory nerves*. Australian Research Council (Australia). Funding: **305,000 €**

2020-2023 **Discovery Projects 2021** (DP210102346): *Topotactic control of magnetism in multiferroic and skyrmion materials*. Australian Research Council (Australia). Funding: **350,000 €**

2021-2022 **Linkage Infrastructure Project** (LE210100086): *A platform for probing nanoscale magnetic states under multiple actuations*. Australian Research Council (Australia). Funding: **390,000 €**

2020-2023 **Linkage Project** (LP190100113): *Engineering nanoionic interfaces towards high performance cathode coatings*. Australian Research Council (Australia). Funding: **338,000 €**

2020-2023 Linkage Project (LP190100829): *High performance metal oxide inks for printable memory arrays*. Australian Research Council (Australia). Funding: **259,000 €**

2020 Faculty Research Grant 2020: *Multiferroic solid solutions for novel magnetoelectric and energy-conversion applications*. UNSW Sydney (Australia). Funding: **10,500 €**

2020 Interdisciplinary Seed Funding Award 2020: *Manipulating hydride and proton ionic conduction towards enabling advanced batteries for energy storage*. UNSW Sydney (Australia). Funding: **24,000 €**

2015-2019 Future Fellowship (FT140100135): *Rational design of novel multiferroic materials for energy harvesting and energy efficiency*. Australian Research Council (Australia). Funding: **623,000 €**

2011-2014 JAE-DOC Fellowship: *Study of multifunctional oxide materials with first-principles simulation techniques*. Consejo Superior de Investigaciones Científicas and European Science Foundation (Spain). Funding: **150,000 €**

Research funding as Partner Investigator

2025-2028 MSCA Staff Exchanges (101183049): *Solar cells-inspired inorganic semiconductor synaptic systems for low energy edge computing and visual learning*. European Research Commission (Europe). Funding: **676,200 €**

2024-2027 Plan Nacional de Investigación Científica y Técnica y de Innovación 2023 (PID2023-146623NB-I00): *Tackling Disorder: The physics behind energy harvesting*. Agencia Estatal de Investigación (Spain). Funding: **172,000 €**

2024-2027 Plan Nacional de Investigación Científica y Técnica y de Innovación 2023 (PID2023-147469NB-C21): *Many-body approaches to quantum matter*. Agencia Estatal de Investigación (Spain). Funding: **206,000 €**

2023-2025 Discovery Projects 2023 (DP230101040): *Bioinspired nanoionic materials for Watt-scale nano-hydroelectric generator*. Australian Research Council (Australia). Funding: **412,000 €**

2021-2023 Plan Nacional de Investigación Científica y Técnica y de Innovación 2020 (PID2020-112975GB-I00): *Disorder as a tool for energy harvesting*. Agencia Estatal de Investigación (Spain). Funding: **230,000 €**

2021-2023 Plan Nacional de Investigación Científica y Técnica y de Innovación 2020 (PID2020-113565GB-C21): *Simulation of quantum ultradilute gases and liquids*. Agencia Estatal de Investigación (Spain). Funding: **90,000 €**

2020-2023 Industry Project: *Combined barocaloric and electrocaloric effects to surpass hysteresis*. TOTAL Energies (France). Funding: **284,000 €**

2020-2024 Training Centre (IC200100023): *ARC training centre for the global hydrogen economy*. Australian Research Council (Australia). Funding: **3,500,000 €**

2018-2020 **Industry Project:** *Enhancing the performance of photovoltaic panels by phase change inhibited materials.* YCGC Pty. Ltd. (Australia). Funding: **81,500 €**

2018-2020 **Industry Project:** *Development of advanced cathode materials for high performance Li-ion batteries.* Qidong QiAo New Materials Technology Co. Ltd. (Australia). Funding: **180,500 €**

PhD and Master theses supervised

2025-present **Gustavo Madrigal**, Universitat Politècnica de Catalunya (Spain), “*First-principles study of fuel conversion catalytic reactions*”, **PhD (in progress)**

2024-present **Ares Sanuy Latorre**, Universitat Politècnica de Catalunya (Spain), “*Atomistic simulation of molecular crystals for energy applications*”, **PhD (in progress)**

2023-present **Pol Benítez Colominas**, Universitat Politècnica de Catalunya (Spain), “*Computational study of novel materials for energy applications*”, **PhD (in progress)**

2022-present **Cibrán López Álvarez**, Universitat Politècnica de Catalunya (Spain), “*First-principles study of low-dimensional photovoltaic materials*”, **PhD (in progress)**

2017-2019 **Arun K. Sagotra**, UNSW Sydney (Australia), “*Computational study of fast-ion conductors under stress*”, **PhD**

2018-2020 **César Menéndez Muñiz**, UNSW Sydney (Australia), “*First-principles study of the functionality of cobalt-based multiferroic oxides*”, **PhD**

2019-2022 **Jonathan Hopkins**, UNSW Sydney (Australia), “*Tailored synthesis of conjugated polymers with phosphonate functionalities for bioelectronic devices*”, **PhD**

2019-2022 **Cam Phu Thi Nguyen**, UNSW Sydney (Australia), “*Nanomechanical characterization of functional materials using scanning probe microscopy*”, **PhD**

2021-2022 **Cibrán López Álvarez**, Universitat Autònoma de Barcelona (Spain), “*A correlation study in fast-ion conductors*”, **Master**

2020-2021 **Zizhen Zhou**, UNSW Sydney (Australia), “*Computational study of oxygen diffusion in SrTiO₃ under external mechanical and electric fields*”, **Master**

2019-2020 **Joel Shenoy**, UNSW Sydney (Australia), “*Mixing thermodynamics and photocatalytic properties of GaP-ZnS solid solutions*”, **Master**

2019-2020 **Wenhan Yi**, UNSW Sydney (Australia), “*The structural and electronic properties of BiVO₄ with several different dopants*”, **Master**

2019-2020 **Ruizhe Chen**, UNSW Sydney (Australia), “*First-principles study of the structure and ionic diffusion mechanism in lanthanum lithium titanate*”, **Master**

Teaching experience

2024-present “*Electromagnetism*”, Universitat Politècnica de Catalunya (**Spain**)

2022-present “*Functional Materials*”, Universitat Politècnica de Catalunya (**Spain**)

2021-present “*Quantum Physics*”, Universitat Politècnica de Catalunya (**Spain**)

2021-present “*Physics I, II*”, Universitat Politècnica de Catalunya (**Spain**)

2020 MATS2001 *"Physical Properties of Materials"*, UNSW Sydney (**Australia**)
 2020 MATS6001 *"Fundamentals Materials Processing"*, UNSW Sydney (**Australia**)
 2020 MATS6008 *"Advanced Functional Materials"*, UNSW Sydney (**Australia**)
 2020 MATS6101 *"Thermodynamics, Phase Equilibria"*, UNSW Sydney (**Australia**)
 2016-2020 MATS3006 *"Design of Materials"*, UNSW Sydney (**Australia**)
 2015-2020 NANO2002/NANO3001 *"Nanotechnology"*, UNSW Sydney (**Australia**)

Organization of international meetings and seminars

2025 *International Meeting on Relaxation in Complex Systems*, Barcelona (**Spain**)
 2021 *Asia Pacific Center for Theoretical Physics: Multiferroics*, Sydney (**Australia**)
 2018 *Australian Symposium: Computationally Materials*, Sydney (**Australia**)
 2018 *Introduction to Machine Learning in Materials Science*, Sydney (**Australia**)
 2017 *Annual Condensed Matter and Materials Meeting*, Wagga Wagga (**Australia**)
 2015-2019 *UNSW Sydney Materials Science Seminars*, Sydney (**Australia**)

Selected invited talks and seminars (last 5 years)

2025 *Fundamentals Physics of Ferroelectrics*, Annapolis (**USA**), *"Giant photocaloric effects across a vast temperature range in ferroelectrics"*
 2024 *Materials Research Society Spring Meeting*, Seattle (**USA**), *"How correlated are ion hoppings in inorganic solid-state electrolytes?"*
 2024 *American Physical Society March Meeting*, Minneapolis (**USA**), *"Excitonic to superconductor phase transition in ultra-compressed helium"*
 2024 XXXIX Biennial of the Royal Spanish Society, San Sebastián (**Spain**), *"Novel caloric effects in ferroelectrics for solid-state cooling applications"*
 2024 *First Asia-Oceania Neutron Scattering Association Symposium: Neutron Scattering Applications for Caloric Materials*, Shenyang (**China**), *"Giant photocaloric effects across a vast temperature range in ferroelectrics"*
 2024 *Fundamentals Physics of Ferroelectrics*, Washington D. C. (**USA**), *"Novel photophononic effects in archetypal ferroelectrics"*
 2023 *International Symposium on Inorganic and Environmental Materials*, Montpellier (**France**), *"Universal ion-transport descriptors of inorganic solid-state electrolytes"*
 2023 *Materials Research Society Spring Meeting*, San Francisco (**USA**), *"Universal ion-transport descriptors and classes of inorganic solid-state electrolytes"*
 2023 ZCAM-ASEVA Metal-oxide ultrathin films and nanostructures, Zaragoza (**Spain**), *"Piezo-photocatalytic materials: What is known and what is ahead"*
 2022 *Fundamentals Physics of Ferroelectrics*, Washington D. C. (**USA**), *"Novel piezoelectric materials for photocatalytic water splitting"*
 2022 *Psi-K Conference*, Lausanne (**Switzerland**), *"High-throughput screening and strain engineering of photocatalytic materials green hydrogen production"*

2021 EFIMAT Workshop: Advanced materials for the efficient use of energy, Valencia (**Spain**), “*Strain Engineering of Photocatalytic Materials*”

2021 2nd Nanotech-Eurasia Conference, Baku (**Azerbaijan**), “*First-principles high-throughput screening of bulk piezo-photocatalytic materials for sunlight-driven hydrogen production*”

2020 International Conference on Nanoscience and Nanotechnology, Brisbane (**Australia**), “*Rational engineering of semiconductors for photocatalytic applications*”

Other merits

2024-present **American Physical Society (APS) Divisional Associate Editor** for the highly prestigious peer-review journal “*Physical Review Letters*”

2021-2022 **French-Australian Research Network on Conversion and Energy Storage**, IRN-FACES, Hydrogen Energy Coordinator

2020-2023 **Hydrogen Energy Research Centre**, UNSW Sydney (Australia), Leader Program “*Advanced Modelling Techniques for Material Development*”

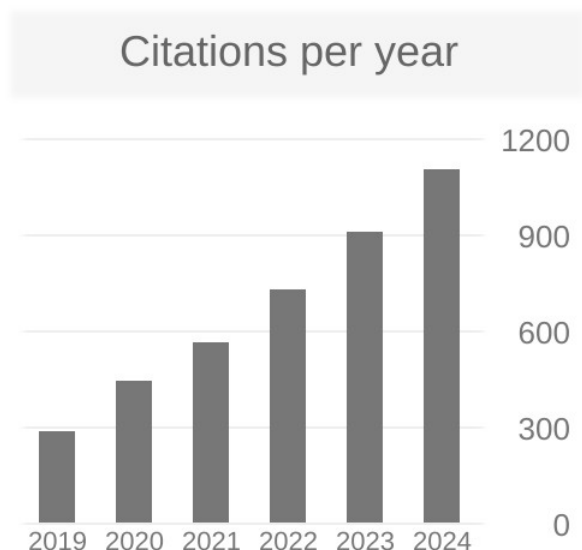
2020 **Guest Editor of Special Issue** “*The Role of Non-Stoichiometry in the Functional Properties of Oxide Materials*”, “*Frontiers in Chemistry*” journal

2018 **Guest Editor of Special Issue** “*Quantum Crystals*”, “*Crystals*” journal

2018-2020 **HPC Pawsey Energy & Resources Allocation Committee** (Australia)

2015-present **Funding Grants Reviewer** for Australian Research Council (**Australia**), Agencia Estatal de Investigación (**Spain**) and National Science Foundation (**USA**)

Publications summary & Citation statistics



- **Consistently ranked within the 2% best researchers** in the field of *Physics & Astronomy* over the last 5 years (<https://topresearcherslist.com/>)
- **>180 peer-reviewed articles:**
 - ~ 35% published in **high-impact factor** (IF >10) journals
 - ~ 65% **first, last or corresponding author**
- ~ **6000 citations**, **h-index: 45**, **i10-index: 132** (*Google Scholar*)

- **Publication portfolio highlights** (~ 85% published over the last 5 years):
1 *Nature*, 1 *Nature Physics*, 6 *Nature Communications*, 2 *Science Advances*, 3 *Advanced Materials*, 1 *Energy & Environmental Science*, 3 *Advanced Energy Materials*, 6 *Advanced Functional Materials*, 2 *Advanced Science*, 3 *Small*, 1 *Angewandte Chemie International Edition*, 2 *ACS Energy Letters*, 2 *Nano Letters*, 1 *ACS Nano*, 3 *Chemistry of Materials*, 2 *Materials Horizons*, 4 *Journal of Materials Chemistry A*, 1 *Reviews of Modern Physics*, 7 *Physical Review Letters*
- **2 book chapters**
- **7 review articles**

Peer-reviewed journal articles (last 5 years)

[90] **Nature Physics** 21, 11 (2025)

C. Cazorla

“A solid-state electrolyte with liquid-like vibrational character”

[89] **ACS Applied Materials & Interfaces** 17, 1428 (2025)

C. Escorihuela-Sayalero, A. Sanuy, L. C. Pardo and C. Cazorla

“Orientational disorder and molecular correlations in hybrid organic-inorganic perovskites: From fundamental insights to technological applications”

[88] **Scientific Reports** 14, 26634 (2024)

J. L. Rodrigo-Ramón, S. Anzellini, C. Cazorla, P. Botella, A. García-Baemud, J. Sánchez-Martín, G. Gasbarino, A. Rosa, S. Gallego-Parra and D. Errandonea

“Thermal equation of state of Rh characterized by XRD in a heated diamond anvil cell”

[87] **Advanced Energy Materials** 14, 2402786 (2025)

C. Wing, C. Cazorla, S. Zhou, D. Zhang, H. Xu, W. Zhong, M. Zhang, D. Chu, Z. Han and R. Amal

“Facet engineering of cobalt manganese oxide for stable oxygen evolution reaction”

[86] **npj 2D Materials and Applications** 8, 64 (2024)

M. Raya-Moreno, C. Cazorla, E. Canadell and R. Rurali

“Phonon transport manipulation in TiSe₂ via reversible charge density wave melting”

[85] **Physical Review Letters** 113, 116401 (2024)

R. Rurali, C. Escorihuela-Sayalero, J. Ll. Tamarit, J. Íñiguez, and C. Cazorla

“Giant photocaloric effects across a vast temperature range in ferroelectric perovskites”

[84] **Physical Review Materials** 8, 094403 (2024)

L. Féger, C. Escorihuela-Sayalero, J.-M. Rampnoux, K. Kontou, J. Íñiguez, C. Cazorla, I. Monot-Laffez, S. Douri, S. Grauby, R. Rurali, S. Dilhare, S. Gomès and G. F. Nataf

“Lead-free room-temperature ferroelectric thermal conductivity switch using anisotropies in thermal conductivities”

[83] **Journal of Open Source Software** 9, 6616 (2024)

C. López, R. Rurali, and C. Cazorla

“IonDiff: command-line tool to identify ionic diffusion events and hopping correlations in molecular dynamics simulations”

[82] **ACS Energy Letters** 9, 3970 (2024)

L. Hu, X. Guan, H. Huang, J. Ding, A. A. Koushik, W. Wang, C.-H. Lin, T. Wan, M. Li, J. Yi, R. Zheng, D. Chu, S. Cai, J. Chen, C. Cazorla, J. Yuan, Y. Bai, T. Wu and S. Huang
“Assessing the optoelectronic performance of halide perovskite quantum dots with identical bandgaps: Composition tuning versus quantum confinement”

[81] **Advanced Functional Materials** 34, 2406678 (2024)

C. López, I. Caño, D. Rovira, P. Benítez, J. M. Asensi, Z. Jehl, J. Ll. Tamarit, E. Saucedo and C. Cazorla

“Machine-learning aided first-principles prediction of earth-abundant pnictogen chalcogenide solid solutions for solar-cell devices”

[80] **Advanced Science** 11, 2306488 (2024)

M. Zeng, C. Escorihuela-Sayalero, T. Ikeshoji, S. Takagi, S. Kim, S. Orimo, M. Barrio, J. Ll. Tamarit, P. Lloveras, C. Cazorla, and K. Sau

“Colossal reversible barocaloric effects in a plastic crystal mediated by lattice vibrations and ion diffusion”

[79] **Nanoscale** 16, 88335 (2024)

C. Cazorla, S. Bichelmaier, C. Escorihuela-Sayalero, J. Íñiguez, J. Carrete, and R. Rurali
“Light-driven dynamical tuning of the thermal conductivity in ferroelectrics”

[78] **Journal of the American Chemical Society** 146, 8269 (2024)

C. López, R. Rurali, and C. Cazorla

“How concerted are ionic hops in inorganic solid-state electrolytes?”

[77] **Journal of Materials Chemistry C** 12, 3154 (2024)

I. Caño, J. Turnley, P. Benítez, C. López, J.-M. Asensi, D. Payno, J. Puigdollers, M. Placidi, C. Cazorla, R. Agrawal and E. Saucedo

“Novel synthesis of semiconductor chalcogenide anti-perovskites by low-temperature molecular precursor ink deposition methodologies”

[76] **Journal of the American Chemical Society** 146, 4913 (2024)

C. Zhao, C. Cazorla, X. Zhang, H. Huang, D. Li, J. Shi, Q. Zhao, W. Ma and J. Yuan

“Fast organic cation-exchange in colloidal perovskite quantum dots towards functional optoelectronic applications”

[75] **npj Computational Materials** 10, 13 (2024)

C. Escorihuela-Sayalero, L. C. Pardo, M. Romanini, N. Obrecht, S. Loehlé, P. Lloveras, J. Ll. Tamarit, and C. Cazorla

“Prediction and understanding of barocaloric effects in orientationally disordered materials from molecular dynamics simulations”

[74] **ACS Applied Materials & Interfaces** 15, 53614 (2023)

Z. Zhou, C. Cazorla, B. Gao, H. D. Luong, T. Momma, and Y. Tateyama

“First-principles study on the interplay of strain and state-of-charge with Li-ion diffusion in the battery cathode material LiCoO₂”

[73] **Physical Review Materials** 7, 113607 (2023)

V. Tuli, P. A. Burr, A. Claisse and C. Cazorla

“Thermodynamic stability of beta-phases in Zr-Nb alloys”

[72] **Physical Review Letters** 131, 189602 (2023)

M. de Koning, W. Cai, C. Cazorla, and J. Boronat

“Reply to Comment on “Absence of off-diagonal long-range order in hcp 4He dislocation cores”

[71] **Cell Reports Physical Science** 4, 101643 (2023)

D. Zhang, C. Tsounis, Z. Ma, L. Peng, Z. Lin, H. Yin, F. Le-Hussain, C. Cazorla, D. Chu, R. Amal and Z. Han

“Enhancing hydrogen peroxide electrosynthesis by manipulating the three-phase interface microenvironment”

[70] **Nature Communications** 14, 6165 (2023)

Y. Chen, L. Soler, C. Cazorla, J. Oliveras, N. G. Bastús, V. Puentes, and J. Llorca

“Facet-engineered TiO₂ drives photocatalytic activity and stability of supported noble metal clusters during H₂ evolution”

[69] **Journal of Materials Chemistry A** 11, 16743 (2023)

D. Kim, J. S. Yun, D. Kim, A. Sagotra, A. Mattoni, P. Sharma, J. Kim, D. Lee, S. Lim, P. O'Reilly, L. Brinkman, M. A. Green, S. Huang, A. Ho-Baillie, C. Cazorla, and J. Seidel

“Charge carrier transport properties of twin domains in halide perovskites”

[68] **Small Structures** 4, 2300194 (2023)

L. Peng, D. Zhang, Z. Ma, D. Chu, C. Cazorla, R. Amal, and Z. Han

“Enhanced hydrogen evolution reactions on Ru/a-Ni-MoO₃ electrocatalysts”

[67] **Nature Communications** 14, 4458 (2023)

C. Liu, I. Errea, C. Pickard, L. J. Conway, B. Monserrat, Y.-W. Fang, C. Ding, Q. Lu, J. Sun, J. Boronat and C. Cazorla

“Excitonic insulator to superconductor phase transition in ultra-compressed helium”

[66] **Physical Chemistry Chemical Physics** 25, 17450 (2023)

C. Menéndez, R. Rurali, and C. Cazorla

“Colossal room-temperature electrocaloric strength aided by hydrostatic pressure in lead-free multiferroic solid solutions”

[65] **Chemistry of Materials** 35, 4882 (2023)

J. Hopkins, K. Fidanovksi, L. Travaglini, D. Ta, J. Hook, P. Wagner, K. K. Wagner, A. Lauto, C. Cazorla, D. L. Officer, and D. Mawad

“Correction to A phosphonated poly(ethylenedioxythiophene) derivative with low oxidation potential for energy-efficient bioelectronic devices”

[64] **Advanced Materials Technologies** 8, 2300777 (2023)

J. Hopkins, D. Ta, A. Lauto, J. Daniels, P. Wagner, N. Kirby, C. Cazorla, and D. Mawad

"Impact of side chain extension on the morphology and electrochemistry of phosphonated poly(ethylenedioxythiophene) derivatives"

[63] **npj Computational Materials** 9, 97 (2023)

C. Cazorla, M. Stengel, J. Íñiguez, and R. Rurali

"Giant multiphononic effects in a perovskite oxide"

[62] **Energy & Environmental Science** 16, 2338 (2023)

R. Zhu, Y. Zhu, L. Hu, P. Guan, D. Su, S. Zhang, C. Liu, Z. Feng, G. Hu, F. Chen, T. Wan, X. Guan, T. Wu, R. Joshi, M. Li, C. Cazorla, Y. Lu, Z. Han, H. Xu, and D. Chu

"Lab free protein-based moisture electric generators with high electric output"

[61] **Materials Science and Technology** 39, 1180 (2023)

P. Guan, Z. Xu, T. Ji, S. Zhang, J. Elliott, T. Wan, C. Cazorla and D. Chu

"The cationic interstitials induced resistive switching: A case study on Mn-doped SnO₂"

[60] **Pharmaceutics** 15, 196 (2023)

S. Valenti, C. Cazorla, M. Romanini, J.-Ll. Tamarit, and R. Macovez

"Eutectic formation and relaxation dynamics of mixtures of two benzodiazepine drugs"

[59] **Materials Horizons** 10, 1757 (2023)

C. López, A. Emperador, E. Saucedo, R. Rurali and C. Cazorla

"Universal ion-transport descriptors and classes of inorganic solid-state electrolytes"

[58] **ACS Sustainable Chemistry & Engineering** 11, 3370 (2023)

Y. Jiang, C. Y. Toe, S. S. Mofarah, C. Cazorla, S. L. Y. Chang, Y. Yin, Q. Zhang, S. Lim, Y. Yao, R. Tian, Y. Wang, H. Arandiyani, J. Scott, P. Koshy, D. Wang and C. C. Sorrell

"Efficient cocatalyst-free piezo-photocatalytic hydrogen evolution of defective BaTiO_{3-x} nanoparticles from seawater"

[57] **Physical Review Letters** 130, 016001 (2023)

M. de Koning, W. Cai, C. Cazorla and J. Boronat

"Absence of off-diagonal long-range order in hcp ⁴He dislocation cores"

[56] **The Journal of Physical Chemistry C** 126, 21453 (2022)

R. Lawrence, Q. Ramasse, D. Sando, C. Cazorla, N. Valanoor and M. Arredondo

"Effects of multiple local environments on EELS of epitaxial perovskite interfaces"

[55] **ACS Sustainable Chemistry & Engineering** 10, 16924 (2022)

Zhao Liu, Biao Wang and Claudio Cazorla

"Strain-engineering of 2D piezo-photocatalytic materials for improved H₂ ERR"

[54] **ACS Energy Letters** 7, 4150 (2022)

L. Hu, X. Guan, T. Wan, C.-H. Lin, S. Liu, R. Zhu, W. Chen, L. Yuan, S. Shahrokhi, C. Cazorla, J. Chen, J. Yang, J. Yi, D. Chu, S. Huang and T. Wu

"Valence-regulated metal doping of mixed-halide perovskites to modulate phase segregation and solar cell performance"

[53] **Journal of Materials Chemistry A** 10, 18132 (2022)

Zhao Liu, Biao Wang, Dewei Chu and Claudio Cazorla

"First-principles high-throughput screening of bulk piezo-photocatalytic materials for sunlight-driven hydrogen production"

[52] **Journal of Colloid and Interface Science** 628, 407 (2022)

P. Guan, Y. Zhu, M. Li, T. Zeng, T. Wan, Y. Liu, C. Cazorla, and D. Chu

"Enhancing cyclic and in-air stability of Ni-rich cathodes"

[51] **The Journal of Physical Chemistry C** 126, 14329 (2022)

M. M. Seyfour, D. Zhang, C. Menéndez, D. Sando, C. Cazorla, J. Seidel and D. Wang

"Engineering photoresponse in epitaxial $\text{BiFe}_{0.5}\text{Cr}_{0.5}\text{O}_3$ thin films"

[50] **ACS Applied Materials & Interfaces** 14, 37009 (2022)

Z. Zhou, D. Chu, B. Gao, T. Momma, Y. Tateyama and C. Cazorla

"Tuning the electronic, ion transport and stability properties of lithium-rich manganese based oxide materials with oxide perovskite coatings"

[49] **Angewandte Chemie International Edition** 61, e202205111 (2022)

C. Han, Y. Wang, J. Yuan, J. Sun, X. Zhang, C. Cazorla, X. Wu and W. Ma

"Tailoring phase alignment and interfaces via polyelectrolytes anchoring enables large-area two-dimensional perovskite solar cells"

[48] **Advanced Energy Materials** 12, 2201469 (2022)

S. Hu, W. Han, X. Li, Y. Ji, Q. Liu, J. Wang, J. He, C. Cazorla, Y. Zhu and L. Chen

"Converting brownmillerite to alternate layers of oxygen-deficient and conductive nano-sheets with enhanced thermoelectric properties"

[47] **The Journal of Physical Chemistry Letters** 13, 5061 (2022)

A. I. Krivchikov, O. O. Romantsova, L. M. Buravtseva, C. Cazorla and J. Ll. Tamarit

"The role of optical phonons and anharmonicity in the appearance of the heat capacity Boson peak-like anomaly in fully ordered molecular crystals"

[46] **Small** 18, 2200847 (2022)

S. Shahrokhi, M. Dubajic, S. Bremner, X.-G. Li, C. Cazorla and T. Wu

"Anomalous structural evolution and glassy lattice in mixed-halide hybrid perovskites"

[45] **Advanced Energy Materials** 12, 2200537 (2022)

J. Guo, J. Sun, L. Hu, S. Fang, X. Ling, X. Zhang, Y. Wang, H. Huang, C. Han, Z. Zhou, C. Cazorla, Y. Yang, D. Chu, T. Wu, J. Yuan and W. Ma

"Indigo: A natural molecular passivator for efficient perovskites solar cells"

[44] **ACS Applied Materials & Interfaces** 14, 16338 (2022)

M. Li, Z. Zhou, L. Hu, S. Wang, Y. Zhou, T. Wan, C. Cazorla, J. Yi and D. Chu

"Hydrazine hydrate intercalated 1T-dominant MoS_2 with superior ambient stability for highly efficient electrocatalytic applications"

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