Sharon Mitchell

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Nationality: British **Date of birth:** 22.04.1982

Education

09/05-10/09	PhD in Materials Chemistry, University of Cambridge, UK Advisor: Prof. William Jones Title: Synthesis and characterization of layered inorganic mixed metal oxides and hydroxides. Awards: EPSRC fellowship
09/00-10/04	MSci in Natural Sciences, University of Cambridge, UK Dissertation: Co-crystallization of chiral active pharmaceutical ingredients by solution and grinding techniques

Professional Appointments

08/20-ongoing	Program advisor and Education officer, NCCR Catalysis, Switzerland
10/18-ongoing	Lecturer, ETH Zurich, Switzerland
05/13-09/18	Scientist, ETH Zurich, Switzerland
03/10-05/13	Postdoctoral researcher, ETH Zurich, Switzerland
05/09-03/10	Postdoctoral researcher, ICIQ, Spain
06/04-01/05	Internship, Johnson Matthey, Royston, UK

Professional Summary

Leveraging 16+ years of experience as a researcher and lecturer, I am passionate about advancing frontiers of catalytic materials design for sustainable chemical synthesis. My journey integrates advanced techniques, emphasizing a profound understanding of structure-performance relationships across relevant scales. I particularly enjoy exploring the integration of machine learning and sustainability tools for experimental research. Expertise include the design of low-nuclearity catalysts, hierarchical pore networks, and multicomponent shaped bodies. Beyond technical realms, I am committed to fostering the growth of the next generation of researchers.

Scientific Output

Over 115 original research, review, and opinion articles, generating over 7605 (9398, 1953 in 2023) citations and an H-index of 45 (48) according to Web of Science (Google Scholar) accessed 23.11.23. >80 proceedings at (inter)national meetings, 11 invited talks, and 2 patents. A complete list of scientific output is appended.

5 Key Publications as (co-)corresponding author

- Reactivity and mechanism of recoverable $Pd_1@C_3N_4$ single-atom catalyst in Buchwald-Hartwig aminations. Giannakakis et al. *ACS Catal.* **2024**, doi:10.1021/acscatal.4c05134.
- Quantitative description of metal center organization and interactions in single atom catalysts. Rossi et al. *Adv. Mater.* **2023**, 36, 2307991.
- Droplet-based microfluidics platform for the synthesis of single-atom heterogeneous catalysts. Moragues et al. *Small Structures* **2023**, 4, 2200284.
- Atomically precise control in the design of low-nuclearity supported metal catalysts. Mitchell and Pérez-Ramírez. *Nat. Rev. Mater.* **2021**, 6, 969.
- Elucidation of metal local environments in single-atom catalysts based on carbon nitrides. Büchele et al. *Small* **2022**, 18, 2202080.

Teaching and Supervision

- Co-lectured 4 courses (3 currently, 2 as main lecturer), guest lectured 2 courses, assisted in 2 courses and supervised 2 practicals in catalysis, materials science, and sustainable chemistry.
- Co-supervised 15 doctoral students (3 currently) and 14 post-doctoral researchers (2 currently).

Funding and Project Management

- Support in the successful securement of competitive funds (one ETH, five SNSF, three EU, and six industrial projects) with Prof. J. Pérez-Ramírez (PI), nine as co-investigator. Amount awarded: 2.5 mCHF.
- Coordinated the preparation of the proposal for Phase I (2020) and Phase II (2024) of NCCR Catalysis, established in August 2020 with a budget of over 30 mCHF per phase.
- Co-applicant of an ETH equipment grant. Amount awarded: 25 kCHF (2019).

Community Engagement

- Part of management team of NCCR Catalysis (Program Advisor and Education Officer), a National Center of Competence in Research funded by the Swiss National Science Foundation, involving 47 Principal Investigators and >200 members.
- Guest editor of the themed issue on Single Atom Catalysis in Catalysis Science and Technology (2017).
- Reviewer in high-ranked journals including Nature Materials, Nature Communications, Chemistry of Materials, Journal of Materials Chemistry, ACS Catalysis, Journal of Catalysis, Catalysis Science and Technology, Applied Catalysis B (ca. 30 per year). Outstanding reviewer for Catalysis Science and Technology in 2018.
- Session chair at (inter)national meetings including EuropaCat (2023) the Advanced Porous Materials Symposium (2014), the CASCATBEL Summer School (2014), and the first SCS Heterogeneous Catalysis Meeting (2011).
- Organizer of the Advanced Porous Materials (2012, 2014) and Materials, Characterization, and Catalysis (2018) workshops in collaboration with Micromeritics Instruments Corporation.
- Co-initiator and coordinator of the ICB Seminar Series (2011-2013).
- Consultant on analytical methods for porosity assessment and advanced visualization tools (2010-ongoing).
- Web Manager for group (2010-ongoing).

Awards

9 best poster prizes at (inter)national meetings (2012, 2014, 2015, 2017, 2019, 2021, 2023), Sidney Sussex College Scientific Travel Grant (2009), Engineering and Physical Sciences Research Council Fellowship (2006).

Languages

English (native), Spanish (conversational), German (conversational), and French (basic).

Full Overview of Teaching Duties, Project Management, and Scientific Output

Teaching

2023-ongoing	Sustainable chemistry and chemical engineering in industry, ETH Zurich, Lecturer (10%, main responsible).
2023-ongoing	Concepts and tools in sustainable chemicals manufacture, ETH Zurich, Lecturer (30%, main responsible).
2018-ongoing	Catalysis engineering, ETH Zurich. Lecturer (30%).
2011-2017	Catalysis engineering, ETH Zurich. Assistant and guest lecturer.
2014	Elements of microscopy, ETH Zurich. Assistant to course (3 classes).
2013	Heterogeneous reaction engineering, ETH Zurich. Lecturer (50%).
2010-2013	Characterization of catalysts and surfaces, ETH Zurich. Guest lecturer (4-8 classes per year).
2006-2009	Chemistry of materials, University of Cambridge. Exercise classes (6-8 h per week).
2006-2008	Techniques in modern synthetic chemistry, University of Cambridge. Practical supervision (4 h per week).
2005-2007	Physical and inorganic chemistry, University of Cambridge. Delivery of practical classes (4 h per week).

Supervision of Doctoral Students

11/24-12/24	Yuguo Dong. Guest student. Single-atom catalysts for biomass transformations.
10/23-ongoing	Yung-Tai Chiang. Novel single-atom catalyst architectures.
09/22-ongoing	Marc Eduard Usteri. Low-nuclearity heterogeneous catalysts for sustainable organic transformations.
04/21-11/24	Vera Giulimondi. Design of nanostructured metal catalysts for acetylene hydrochlorination.
11/20-12/24	Thomas Moragues. Intelligent synthesis of single atoms catalysts using droplet-based microfluidics. Joint PhD student with Prof. Andrew deMello, ETH Zurich.
09/20-11/24	Dario Poier. Single-atom catalysis – Scope and industrial applications. Joint PhD student with Prof. Roger Marti, HES-SO.
11/19-10/23	Dario Faust Akl. Single atom and low-nuclearity catalysts for sustainable organic synthesis.
07/19-07/21	Alessia Cesarini. Methyl halide coupling for olefins production from natural gas.
10/17-11/21	Simon Büchele. Nuclearity effects in selective catalytic reductions.
09/16-03/18	Ferdy Coumans. Design of continuous heterogeneously-catalysed process for vitamin syntheses.
10/15-01/20	Evgeniya Vorobyeva. Carbon nitride as a platform for single-atom catalysis.
01/15-12/15	Sundararajan Thirumalai. Rationalization of additive impacts in technical zeolite catalysts through advanced visualization.
09/10-02/15	Nina-Luisa Michels. From powder to technical body: Structured zeolite catalysts.
08/10-12/14	Maria Milina. Property-function interplay in the design of hierarchical zeolite catalysts.
10/08-06/09	Almudena Gómez Avilés. Visiting PhD student. Synthesis and characterization of layered transition metal molybdates.

Supervision of Postdoctoral Researchers

10/24-ongoing	Dr. Jianyang Wang. Novel architectures of reducible oxide catalysts for green methanol synthesis.
04/23-06/24	Dr. Matteo Vanni. Coke deposition in hierarchical pore structures.
10/22-09/23	Dr. Kevin Rossi. Machine learning for atom detection via image analysis.
10/21-02/24	Dr. Georgios Giannakakis. Single-atom catalysts for Buchwald Hartwig coupling.

07/18-06/19 Dr. Ronghe Lin. Design of a continuous heterogeneously-catalyzed process for vitamin syntheses.

02/16-12/19 Dr. Zupeng Chen. Design of single-atom heterogeneous catalysts based on carbon nitride.

03/15-12/16 Dr. Asier Zubiaga. Structural analysis of porous catalysts by positron annihilation spectroscopy.

02/15-09/16 Dr. Jiaxu Liu. Design of coke-resistant zeolite catalysts for olefin production by alkene cracking.

01/15-12/18 Dr. Robbie Warringham. Structural analysis of porous catalysts by positron annihilation spectroscopy.

01/15-01/16 Dr. Marilyne Boltz. Decoupling the impact of crystal size and morphology on the stability of zeolites in coke-forming reactions.

10/14-09/15 Dr. Zhen Guo. Styrene production over zeolite-based catalysts.

02/13-02/15 Dr. Elodie Rodrigues. Design of mild base catalysts for the deoxygenation of bio-oil by aldol condensation.

11/13-11/14 Dr. Manuel Hernandez-Rodriguez. Origin of acidity changes in hierarchical zeolites.

11/13-11/14 Dr. Lars Borchardt. Structuring zeolite bodies for enhanced heat-transfer properties.

Project Management

09/21-ongoing Co-principal scientist of NCCR Catalysis project: Smart characterization of heterogeneous catalysts

09/21-ongoing Co-principal scientist of NCCR Catalysis project: Deep-learning for microscopy image analysis of low-nuclearity catalysts

09/21-12/24 Co-principal scientist of project of project with Roche: Heterogeneous single-atom palladium catalysis for C-N coupling application.

08/20-ongoing NCCR Catalysis project: Design of low-nuclearity catalysts

03/19-03/20 Co-principal scientist of EU project: Energy-X.

06/17-05/19 Exploratory cooperation with Idorsia Pharmaceuticals Ltd: Evaluation of single-site catalysts in continuous flow organic reactions.

11/16-04/20 Co-principal scientist of project with DSM Nutritional Products: Design of continuous heterogeneously-catalysed process for vitamin syntheses.

10/16-10/19 SNSF project (#200021-169679): Doing more with less: efficient single-atom catalysts for sustainable chemical transformations.

12/15-05/16 Co-principal scientist of project with Zeochem AG: Advanced visualization of technical sorbents.

11/15-03/20 ETH project (#33-15-1): Advanced catalyst engineering with positron annihilation spectroscopy.

10/14-09/16 Co-principal scientist with thyssenkrupp Industrial Solutions: Styrene production over zeolite-based catalysts.

11/13-12/14 Coinvestigator of EU project (#604307): Cascade deoxygenation process using tailored nanocatalysts for the production of biofuels from lignocellullosic biomass.

05/13-04/15 Coinvestigator of European Institute of Innovation and Technology project: CO_2 based products - from dream to reality.

03/11-04/12 Industrial project with BASF: The catalytic conversion of methanol to olefin over desilicated ZSM-5 zeolites.

04/11-09/14 SNSF project (200021-134572): A fundamental approach to the scale up of hierarchical zeolite catalysts.

Peer-Reviewed Articles (* denotes co-corresponding author)

129. G. Giannakakis, M.-E. Usteri, A. Bugaev, A. Ruiz-Ferrando, D. Faust Akl, N. Lopez, S. Fantasia, K. Püntener, J. Pérez-Ramírez, S. Mitchell*. Reactivity and mechanism of recoverable $Pd_1@C_3N_4$ single-atom catalyst in Buchwald-Hartwig aminations. *ACS Catal.* **2024**, doi:10.1021/acscatal.4c05134.
128. H. Eliasson, A. Lothian, I. Surin, S. Mitchell, J. Pérez-Ramírez, R. Erni. Precise size determination of supported catalyst nanoparticles via generative AI and scanning transmission electron microscopy. *Small Methods* **2024**, doi:10.1002/smtd.202401108.
127. M. Agrachev, V. Giulimondi, I. Surin, S. Mitchell, G. Jeschke, J. Pérez-Ramírez. Electron paramagnetic resonance spectroscopy for the analysis of single-atom catalysts. *Chem Catal.* **2024**, *4*, 101136.
126. T. Pinheiro Araújo, S. Mitchell, J. Pérez-Ramírez. Design principles of catalytic materials for CO_2 hydrogenation to methanol. *Adv. Mater.* **2024**, in press (doi:10.1002/adma.202409322).
125. V. Giulimondi, M. Vanni, S. Damir, T. Zou, S. Mitchell, F. Krumeich, A. Ruiz-Ferrando, N. López, J.J. Gata-Cuesta, G. Guillén-Gosálbez, J.J. Smit, P. Johnston, J. Pérez-Ramírez. Convergent active site evolution in platinum single atom catalysts for acetylene hydrochlorination and implications for toxicity minimization. *ACS Catal.* **2024**, *14*, 13652-13664.
124. M.E. Usteri, G. Giannakakis, A. Bugaev, J. Pérez-Ramírez, S. Mitchell*. Understanding and controlling reactivity patterns of $Pd_1@C_3N_4$-catalyzed Suzuki-Miyaura couplings. *ACS Catal.* **2024**, *14*, 12635-12646.
123. E. Lucas, A.J. Martín, S. Mitchell, A. Nabera, L.F. Santos, J. Pérez-Ramírez, G. Guillén-Gosálbez. The need to integrate mass- and energy-based metrics with life cycle impacts for sustainable chemicals manufacture. *Green Chem.* **2024**, *26*, 9300-9309.
122. S. Mitchell, A.J. Martín, G. Guillén-Gosálbez, J. Pérez-Ramírez. The future of chemical sciences is sustainable. *Angew. Chem. Int. Ed.* **2024**, *63*, e202318676. *Angew. Chem.* **2024**, *136*, e202318676.
121. T. Moragues, G. Giannakakis, A. Ruiz-Ferrando, N. López, C.N. Borca, T. Huthwelker, A. Bugaev, A.J. deMello, J. Pérez-Ramírez, S. Mitchell*, Droplet-based microfluidics reveals insights into cross-coupling mechanisms over single-atom heterogeneous catalysts. *Angew. Chem. Int. Ed.* **2024**, *63*, e202401056. *Angew. Chem.* **2024**, *136*, e202406901.
120. T. Pinheiro Araújo, G. Giannakakis, J. Morales-Vidal, M. Agrachev, Z. Ruiz-Bernal, P. Preikschas, T. Zou, F. Krumeich, P.O. Willi, W.J. Stark, R.N. Grass, G. Jeschke, S. Mitchell, N. López, J. Pérez-Ramírez. Low-nuclearity $CuZn_x$ ensembles on $ZnZrO_x$ catalyze methanol synthesis from CO_2. *Nat. Commun.* **2024**, *15*, 3101.
119. T. Zou, T. Pinheiro Araújo, M. Agrachev, X. Jin, F. Krumeich, G. Jeschke, S. Mitchell, J. Pérez-Ramírez. Design of technical ZnO/ZrO_2 catalysts for CO_2 hydrogenation to methanol. *J. Catal.* **2024**, *430*, 115344.
118. Z. Zhang, M. Vanni, X. Wu, P. Hemberger, A. Bodi, S. Mitchell, J. Pérez-Ramírez. CO cofeeding affects product distribution in CH_3Cl coupling over ZSM-5 zeolite: Pressure twists the plot. *Angew. Chem. Int. Ed.* **2024**, *63*, e202401060. *Angew. Chem.* **2024**, *136*, e202401060.
117. D. Poier, D. Faust Akl, E. Lucas, A. Rodrigues Machado, G. Giannakakis, S. Mitchell*, G. Guillén-Gosálbez, R. Marti, J. Pérez-Ramírez. Reaction environment design for multigram synthesis via Sonogashira coupling over heterogeneous palladium single-atom catalysts. *ACS Sustain. Chem. Eng.* **2023**, *11*, 16935-16945.
116. M. Suvarna, A. Claude Vaucher, S. Mitchell, T. Laino, J. Pérez-Ramírez. Language models and protocol standardization guidelines for accelerating synthesis planning in heterogeneous catalysis. *Nat. Commun.* **2023**, *14*, 7964.
115. K. Rossi, A. Ruiz-Ferrando, D. Faust Akl, V. Gimenez Abalos, J. Heras-Domingo, R. Graux, X. Hai, J. Lu, D. Garcia-Gasulla, N. López, J. Pérez-Ramírez, S. Mitchell*. Quantitative description of metal center organization and interactions in single atom catalysts. *Adv. Mater.* **2023**, *36*, 2307991.

114. S. Mitchell, A.J. Martín, J. Pérez-Ramírez. Transcending scales in catalysis for sustainable development. *Nat. Chem. Eng.* **2024**, *1*, 13-15.
113. X. Hai, Y. Zheng, Q. Yu, N. Guo, S. Xi, X. Zhao, S. Mitchell, X. Luo, V. Tulus, M. Wang, X. Sheng, L. Ren, X. Long, J. Li, P. He, H. Lin, Y. Cui, X. Peng, J. Shi, J. Wu, C. Zhang, R. Zou, G. Guillén-Gosálbez, J. Pérez-Ramírez, M.J. Koh, Y. Zhu, J. Li, J. Lu. Geminal atom catalysis for cross-coupling. *Nature* **2023**, *622*, 754-760.
112. X. Li, S. Mitchell, Y. Fang, J. Li, J. Pérez-Ramírez, J. Lu. Recent advances in heterogeneous single-cluster catalysis. *Nat. Rev. Chem.* **2023**, *7*, 754-767.
111. T. Pinheiro Araújo, J. Morales-Vidal, G. Giannakakis, C. Mondelli, H. Eliasson, R. Erni, J.A. Stewart, S. Mitchell, N. López, J. Pérez-Ramírez. Reaction-induced metal-metal oxide interactions in Pd-In_2O_3/ZrO_2 catalysts drive selective and stable CO_2 hydrogenation to methanol. *Angew. Chem. Int. Ed.* **2023**, *62*, e202306563. *Angew. Chem.* **2023**, *42*, e202310340
110. M. Vanni, V. Giulimondi, A. Ruiz-Ferrando, F. Krumeich, A. Clark, S. Mitchell, N. Lopez, J. Pérez-Ramírez. Selectivity control in palladium-catalyzed CH_2Br_2 hydrodebromination on carbon-based materials by nuclearity and support engineering. *ACS Catal.* **2023**, *13*, 5828-5840.
109. D. Faust Akl, G. Giannakakis, A. Ruiz-Ferrando, M. Agrachev, J.D. Medrano-García, G. Guillén-Gosálbez, G. Jeschke, A.H. Clark, O.V. Safonova, S. Mitchell, N. López, J. Pérez-Ramírez. Reaction-induced formation of stable mononuclear Cu(I)Cl species on carbon for low-footprint vinyl chloride production. *Adv. Mater.* **2023**, *35*, 2211464.
108. I. Surin, Z. Tang, J. Geiger, S. Damir, H. Eliasson, M. Agrachev, F. Krumeich, S. Mitchell, V.A. Kondratenko, E.V. Kondratenko, G. Jeschke, R. Erni, N. López, J. Pérez-Ramírez. Low-valent manganese atoms stabilized on ceria for nitrous oxide synthesis. *Adv. Mater.* **2023**, *35*, 2211260.
107. V. Giulimondi, S. Mitchell*, J. Pérez-Ramírez. Challenges and opportunities in engineering the electronic structure of single-atom catalysts. *ACS Catal.* **2023**, *13*, 2981-2997.
106. T. Moragues, S. Mitchell*, D. Faust Akl, J. Pérez-Ramírez, A. deMello. Droplet-based microfluidics platform for the synthesis of single-atom heterogeneous catalysts. *Small Structures* **2023**, *4*, 2200284.
105. T. Pinheiro Araújo, J. Morales-Vidal, T. Zou, M. Agrachev, S. Verstraeten, P.O. Willi, R.N. Grass, G. Jeschke, S. Mitchell, N. López, J. Pérez-Ramírez. Design of flame-made $ZnZrO_x$ catalysts for sustainable methanol synthesis from CO_2. *Adv. Energy Mater.* **2023**, *13*, 2204122.
104. T.P. Araújo, C. Mondelli, M. Agrachev, T. Zou, P.O. Willi, K.M. Engel, R.N. Grass, W.J. Stark, O.V. Safonova, G. Jeschke, S. Mitchell, J. Pérez-Ramírez. Flame-made ternary Pd-In_2O_3-ZrO_2 catalyst with enhanced oxygen vacancy generation for CO_2 hydrogenation to methanol. *Nat. Commun.* **2022**, *13*, 5610.
103. A.J. Martín, S. Mitchell, C. Mondelli, S. Jaydev, J. Pérez-Ramírez. Unifying views on catalyst deactivation. *Nat. Catal.* **2022**, *5*, 854-866.
102. E. Zhao, M. Li, B. Xu, X. Wang, Y. Jing, D. Ma, S. Mitchell, J. Pérez-Ramírez, Z. Chen. Transfer hydrogenation with a carbon-nitride-supported palladium single-atom photocatalyst and water as a proton source. *Angew. Chem. Int. Ed.* **2022**, *61*, e202207410. *Angew. Chem.* **2020**, *134*, e202207410.
101. D. Faust Akl, D. Poier, S.C. D'Angelo, T.P. Araújo, V. Tulus, O.V. Safonova, S. Mitchell*, R. Marti, G. Guillén-Gosálbez, J. Pérez-Ramírez. Assessing the environmental benefit of palladium-based single-atom heterogeneous catalysts for Sonogashira coupling. *Green Chem.* **2022**, *24*, 6879-6888.
100. S. Büchele, A. Yakimov, S.M. Collins, A. Ruiz-Ferrando, Z. Chen, E. Willinger, D.M. Kepaptsoglou, Q.M. Ramasse, C.R. Müller, O.V. Safonova, N. López, C. Copéret, J. Pérez-Ramírez, S. Mitchell*. Elucidation of metal local environments in single-atom catalysts based on carbon nitrides. *Small* **2022**, *18*, 2202080.
99. A. Cesarini, S. Mitchell, G. Zichittella, M. Agrachev, S.P. Schmid, G. Jeschke, Z. Pan, A. Bodi, P. Hemberger, J. Pérez-Ramírez. Elucidation of radical- and oxygenate-driven paths in zeolite-

catalyzed conversion of methanol and methyl chloride to hydrocarbons. *Nat. Catal.* **2022**, *5*, 605-614.

98. S. Mitchell*, F. Parés, D. Faust Akl, S. Collins, D. Kepaptsoglou, Q. Ramasse, D. Garcia-Gasulla, J. Pérez-Ramírez, N. López. Automated image analysis for single-atom detection in catalytic materials by transmission electron microscopy. *J. Am. Chem. Soc.* **2022**, *144*, 8018-8029.
97. G. Giannakakis, S. Mitchell, J. Pérez-Ramírez. Single-atom heterogeneous catalysts for sustainable organic synthesis. *Trends Chem.* **2022**, *4*, 264-276
96. K. Tu, S. Büchele, S. Mitchell, L. Stricker, C. Liu, C. Goldhahn, J. Allaz, Y. Ding, R. Günther, Z. Zhang, J. Sun, S. Stucki, G. Panzarasa, S. Zeeman, I. Burgert, J. Pérez-Ramírez, T. Keplinger. Natural wood-based catalytic membrane microreactors for continuous hydrogen generation. *ACS Appl. Mater. Interfaces* **2022**, *14*, 8417-8426.
95. V. Giulimondi, S.K. Kaiser, M. Agrachev, F. Krumeich, A.H. Clark, S. Mitchell, G. Jeschke, J. Pérez-Ramírez. Redispersion strategy for high-loading carbon-supported metal catalysts with controlled nuclearity. *J. Mater. Chem. A* **2022**, *10*, 5953-5961.
94. A.J. Saadun, S. Mitchell, H. Bonchev, J. Pérez-Ramírez. Carbon-supported bimetallic ruthenium-iridium catalysts for selective and stable hydrodebromination of dibromomethane. *ChemCatChem* **2022**, *14*, e202101494.
93. X. Hai, S. Xi, S. Mitchell, K. Harrath, H. Xu, D. Faust Akl, D. Kong, J. Li, Z. Li, T. Sun, H. Yang, Y. Cui, C. Su, X. Zhao, J. Li, J. Pérez-Ramírez, J. Lu. Scalable two-step annealing method for preparing ultra-high-density single-atom catalyst libraries. *Nat. Nanotechnol.* **2022**, *17*, 174-181.
92. S. Mitchell*, J. Pérez-Ramírez. Atomically precise control in the design of low-nuclearity supported metal catalysts. *Nat. Rev. Mater.* **2021**, *6*, 969-985.
91. D. Faust Akl, A. Ruiz-Ferrando, E. Fako, R. Hauert, O. Safonova, S. Mitchell*, N. López, J. Pérez-Ramírez. Precursor nuclearity and ligand effects in atomically-dispersed heterogeneous iron catalysts for alkyne semi-hydrogenation. *ChemCatChem* **2021**, *13*, 3247-3256.
90. S. Büchele, G. Zichittella, S. Kanatakis, S. Mitchell, J. Pérez-Ramírez. Impact of heteroatom speciation on the activity and stability of carbon-based catalysts for propane dehydrogenation. *ChemCatChem* **2021**, *13*, 2599-2608.
89. S. Mitchell, R. Qin, N. Zheng, J. Pérez-Ramírez. Nanoscale engineering of catalytic materials for sustainable technologies. *Nat. Nanotechnol.* **2021**, *16*, 129-139.
88. T. Sun, S. Mitchell, J. Li, P. Lyu, X.B. Wu, J. Pérez-Ramírez, J. Lu. Design of local atomic environments in single-atom electrocatalysts for renewable energy conversions. *Adv. Mater.* **2021**, *33*, 2003075.
87. S.K. Kaiser, Z. Chen, D. Faust Akl, S. Mitchell, J. Pérez-Ramírez. Single-atom heterogeneous catalysts across the periodic table. *Chem. Rev.* **2020**, *120*, 11703-11809.
86. E. Vorobyeva, V.C. Gerken, S. Mitchell*, A. Sabadell-Rendón, R. Hauert, S. Xi, A. Borgna, D. Klose, S.M. Collins, P.A. Midgley, D.M. Kepaptsoglou, Q.M. Ramasse, A. Ruiz-Ferrando, E. Fako, M.A. Ortuño, N. López, E.M. Carreira, J. Pérez-Ramírez. Activation of copper species on carbon nitride for enhanced activity in the arylation of amines. *ACS Catal.* **2020**, *10*, 11069-11080.
85. S. Büchele, Z. Chen, E. Fako, F. Krumeich, R. Hauert, O.V. Safonova, N. López, S. Mitchell*, J. Pérez-Ramírez. Carrier induced modification of palladium nanoparticles on porous boron nitride for alkyne semi-hydrogenation. *Angew. Chem. Int. Ed.* **2020**, *59*, 19639-19644; *Angew. Chem.* **2020**, *139*, 19807-19812.
84. R. Lin, S. Mitchell*, T. Netscher, J. Medlock, R.T. Stemmler, W. Bonrath, U. Létinois, J. Pérez Ramírez. Substrate substitution effects in the Fries rearrangement of aryl esters over zeolite catalysts. *Catal. Sci. Technol.* **2020**, *10*, 4282-4292.
83. S. Büchele, A.J. Martín, S. Mitchell, F. Krumeich, S.M. Collins, S. Xi, A. Borgna, J. Pérez-Ramírez. Structure sensitivity and evolution of nickel-bearing nitrogen-doped carbons in the electrochemical reduction of CO_2. *ACS Catal.* **2020**, *10*, 3444-3454.

82. S.K. Kaiser, K.S. Song, S. Mitchell, A. Coskun, J. Pérez-Ramírez. Nitrogen-doped carbons with hierarchical porosity via chemical blowing towards long-lived metal-free catalysts for acetylene hydrochlorination. *ChemCatChem* **2020**, *12*, 1922-1925.
81. V. Paunović, S. Mitchell, R. Verel, S.S. Lee, J. Pérez-Ramírez. Aluminum redistribution in ZSM-5 zeolite upon interaction with gaseous halogens and hydrogen halides and implications in catalysis. *J. Phys. Chem. C* **2020**, *1*, 722-733.
80. M. Scharfe, V. Paunović, S. Mitchell, R. Hauert, S. Xi, A. Borgna, J. Pérez-Ramírez. Dual catalyst system for selective vinyl chloride production via ethene oxychlorination. *Catal. Sci. Technol.* **2020**, *10*, 560-575.
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Other Publications

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Patents

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Software and Codes

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Invited Talks

11. S. Mitchell, J. Pérez-Ramírez. Tracking Reactive Intermediates in Zeolite-Catalyzed Hydrocarbon Transformations. Keynote. ACS Spring Meeting, 27 March **2023**, Indianapolis, USA.
10. S. Mitchell, A. Ruiz-Ferrando, K. Rossi. Barcelona Supercomputing Center. 9 March **2023**, Barcelona, Spain.
9. S. Mitchell, J. Pérez-Ramírez. Atomically-precise design of low-nuclearity catalysts. 09 November **2022**, NUS, Singapore.
8. S. Mitchell, J. Pérez-Ramírez. Atomically-precise design of low-nuclearity catalysts. Keynote. DPG Conference, 05 September **2022**, Regensburg, Germany.
7. S. Mitchell, J. Pérez-Ramírez. Analysis of pore quality in hierarchical zeolite catalysts. Hierarchically-ordered materials: From theory to applications workshop, 02 October **2019**, Erlangen, Germany.
6. S. Mitchell, J. Pérez-Ramírez. Assessment of complex pore networks through positron annihilation lifetime spectroscopy. MC2 workshop, 15 January **2018**, ETH Zurich, Switzerland.
5. S. Mitchell, J. Pérez-Ramírez. Innovative methods for the assessment of complex pore networks in catalysts, Materials Chemistry Symposium, 28 September **2017**, University of Cambridge, UK.
4. S. Mitchell, J. Pérez-Ramírez. Role of visualization in the design of hierarchical zeolite catalysts, ScopeM Annual Meeting, 15 April 2015, ETH Zurich, Switzerland.
3. S. Mitchell, J. Pérez-Ramírez. Catalysis of Biomass Summer School, 9 June **2014**, Czech Republic.
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Conference Proceedings

83. G. Giannakakis, S. Fantasia, S. Mitchell*, K. Puentener, J. Pérez-Ramírez. Efficient C-N cross couplings via heterogeneous single-atom catalysis. Talk. Roche TIS Forum, Basel, 28 September **2023**.
82. I. Surin, Z. Tang, J. Geiger, S. Damir, H. Eliasson, M. Agrachev, F. Krumeich, S. Mitchell, V. A. Kondratenko, E. V. Kondratenko, G. Jeschke, R. Erni, N. López, J. Pérez-Ramírez. Talk, Europacat, Prague, 28 August **2023**.

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