doi:10.2533/chimia.2025.359 Chimia 79 (2025) 359–360

Swiss Science Concentrates

A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

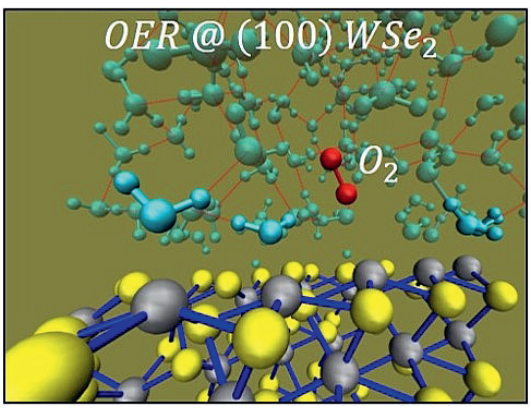
DFT-metadynamics insights on the origin of the oxygen evolution kinetics at the (100)-WSe2 surface

Fabrizio Creazzo[a], Kevin Sivula[b], and Sandra Luber[a]*

iScience **2025**, *28*, 112045
https://doi.org/10.1016/j.isci.2025.112045
[a]Department of Chemistry, University of Zurich, Zurich, Switzerland; [b]Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne, Station 6, CH-1015 Lausanne, Switzerland.

The work from Creazzo, Sivula and Luber investigates the oxygen evolution reaction (OER) on the (100) surface of tungsten diselenide (WSe_2) using density functional theory (DFT) coupled with metadynamics simulations. The OER is a critical but slow step in electrochemical water splitting, which is essential for the hydrogen production. WSe_2, a layered transition metal dichalcogenide, is emerging as a promising non-precious electrocatalyst due to its stability and activity. The study focuses on the understanding of reaction mechanisms, free energy barriers, and the role of the aqueous environment in the OER process. The aqueous environment acts as a co-catalyst significantly enhancing the OER kinetics on WSe_2 by lowering free energy barriers and enabling a water-assisted mechanism. This work provides a deeper understanding of the OER process beyond static calculations and offers a framework for optimising WSe_2-based catalysts for electrochemical water splitting. The results also highlight the importance of including explicit solvent models in DFT-based computational studies of electrocatalytic reactions.

Authors' comments:
"We offer deeper and more realistic insights into OER mechanisms and free energy barriers by overcoming traditional static DFT approaches, also highlighting the crucial role of an explicit modelling of the aqueous environment and providing a framework for targeted optimization of WSe_2-based electrocatalysts for water splitting."



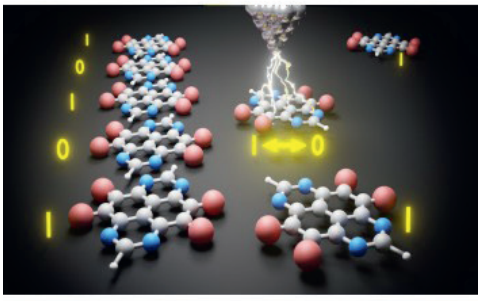
Individual Assembly of Radical Molecules on Superconductors: Demonstrating Quantum Spin Behavior and Bistable Charge Rearrangement

Chao Li, Vladislav Pokorný, Martin Žonda, Jung-Ching Liu, Ping Zhou, Outhmane Chahib, Thilo Glatzel, Robert Häner, Silvio Decurtins, Shi-Xia Liu, Rémy Pawlak, and Ernst Meyer*

ACS Nano **2025**, *19*, 3403
https://doi.org/10.1021/acsnano.4c12387
Department of Physics, University of Basel, CH-4056 Basel, Switzerland; Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, 121 16 Prague 2, Czech Republic; Department of Chemistry, Biochemistry and Pharmaceutical Sciences, W. Inäbnit Laboratory for Molecular Quantum Materials, University of Bern, CH-3012 Bern, Switzerland

This paper investigates the assembly of radical molecules on superconducting surfaces and their quantum spin behaviour. Using scanning tunnelling microscopy, the researchers demonstrated that these molecules can host single-electron spin states and transition between singlet and doublet ground states. The study also explores the emergence of Yu-Shiba-Rusinov states in molecular dimers and chains, confirming theoretical models of superconducting impurities. Especially the molecular chains were of interest because their charge and spin distributions depended on chain length. Odd-numbered chains exhibited a periodic arrangement of charged and neutral molecules, while even-numbered chains formed bistable dimer structures at one end, leading to a frustrated charge configuration. This dimer could be transferred to the other end using an STM tip, demonstrating a controllable mechanism for molecular-scale information storage. These findings pave the way for new approaches in quantum computing and nanoscale superconducting devices.

Authors' comments:
"The various assemblies of TBTAP molecules serve as highly tuneable building blocks, offering significant potential for advancing superconducting molecular quantum technologies."



Cesare Berton, James Southwell, Jonas Genz, Stanislav Prytuliak, Fan Liu, Eda Nisli, Deborah Bäcker, Perle Hermant, Samy Kichou, Dominik Ernst, Tiago Rosa de Araujo, Liam Wenger, Ian Saxer, Henrik Braband, and Jason P. Holland*
Do you want your article to appear in the SWISS SCIENCE CONCENTRATES highlight?
Please contact jason.holland@chem.uzh.ch

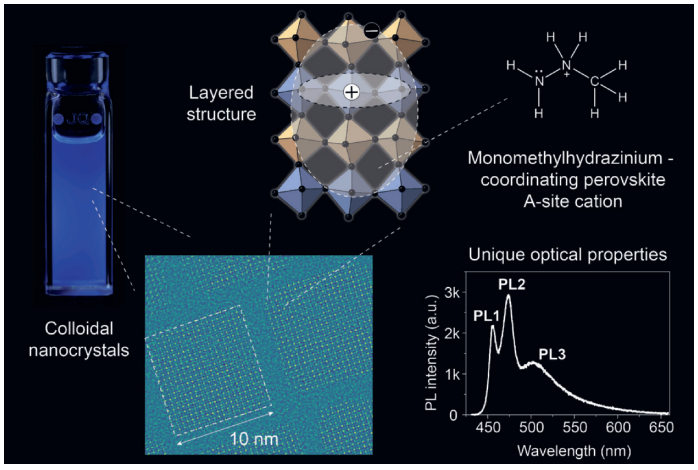
Highly Emissive Colloidal Nanocrystals of a "2.5-Dimensional" Monomethylhydrazinium Lead Bromide

Viktoriia Morad, Taehee Kim, Sebastian Sabisch, Simon C. Boehme, Simone Delessert, Nadine J. Schrenker, Sara Bals, Gabriele Raino, and Maksym V. Kovalenko*

J. Am. Chem. Soc. **2025**, *147*, 6795
https://doi.org/10.1021/jacs.4c16698
Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich CH-8093, Switzerland; Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, Dübendorf CH-8600, Switzerland.

This study explores a novel lead halide perovskite (LHP), monomethylhydrazinium lead bromide ($MMHPbBr_3$), which exhibits a unique '2.5-dimensional' electronic structure. While extending in all three spatial dimensions, its excitonic properties lie between those of 2D and 3D LHPs. Density functional theory (DFT) calculations reveal spatially separated electron and hole wave functions, with electrons delocalized in 3D and holes confined in 2D monolayers. Synthesized through a rapid colloidal method, these nanocrystals (NCs) were characterized using 4D-STEM and nuclear magnetic resonance, confirming their monoclinic structure. Optical analysis demonstrated size-dependent properties and 3D quantum confinement effects, with three distinct photoluminescence (PL) bands at cryogenic temperatures linked to varying interlayer coupling. Single-NC PL spectroscopy further revealed unique photon emission characteristics. These findings contribute to the expansion of exciton engineering in nanomaterials, with potential applications in optoelectronics and quantum technologies.

Authors' comments:
"We investigate pathways towards exotic interlayer excitonic physics in solution-processable lead halide perovskites. For this, we pick a fascinating composition with monomethylhydrazinium, where this coordinating organic cation templates the layered, yet corner-sharing 3D perovskite structure."



A C–H Arylation-Based Enantioselective Synthesis of Planar Chiral Cyclophanes

Soohee Huh, Elvira Linne, Lilian Estaque, Grégory Pieters, Michael Devereux, and Olivier Baudoin*

Angew. Chem. Int. Ed. **2025**, e202500653
https://doi.org/10.1002/ange.202500653
University of Basel, Department of Chemistry, St. Johanns-Ring 19, CH-4056 Basel, Switzerland.

Planar chiral macrocyclophanes are valuable in host–guest chemistry, catalysis, and optoelectronics however controlling their planar chirality remains challenging. This study introduces the first Pd(0)-catalyzed enantioselective intermolecular C–H arylation, enabling the efficient synthesis of planar chiral macrocyclophanes *via* dynamic kinetic resolution. Using chiral, bifunctional phosphine-carboxylate ligands, the researchers achieved high enantioselectivities without the need for directing groups. Mechanistic studies revealed that C–H activation is the enantio determining step, while oxidative addition is reversible, with an inverse isotope effect offering a potential route to improved selectivity. The method successfully generated a wide range of perfluorinated macrocyclophanes and was extended to double C–H arylation from dibrominated precursors. The resulting cyclophanes exhibited interesting chiroptical and photophysical properties, including enhanced circularly polarized luminescence, making them promising candidates for advanced optoelectronic materials.

Authors' comments:
"C–H activation is an efficient tool to control all kinds of stereogenic elements. After centers, axes, and helices, stereogenic planes were the next frontier for us to reach!"