doi:10.2533/chimia.2024.556 Chimia 78 (2024) 556–557

Swiss Science Concentrates

A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

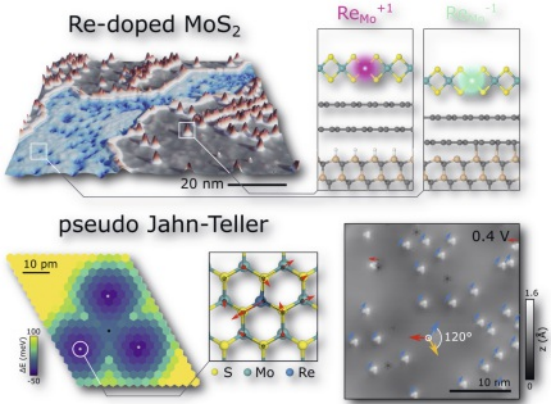
Charge State-dependent Symmetry Breaking of Atomic Defects in Transition Metal Dichalcogenides

Feifei Xiang, Lysander Huberich, Preston A. Vargas, Riccardo Torsi, Jonas Allerbeck, Anne Marie Z. Tan, Chengye Dong, Pascal Ruffieux, Roman Fasel, Oliver Gröning, Yu-Chuan Lin Richard G. Hennig, Joshua A. Robinson, and Bruno Schuler*

Nat. Commun. **2024**, *15*, 2738.
https://doi.org/10.1038/s41467-024-47039-4
Empa – Swiss Federal Laboratories for Materials Science and Technology, Switzerland; University of Florida, USA; The Pennsylvania State University, USA; Institute of High Performance Computing, Singapore; National Yang Ming Chiao Tung University, Taiwan.

Atomic quantum emitters, crucial components in nanophotonics and quantum computing, derive their functionality from host lattice coordination. Alterations in lattice symmetry profoundly impact their optical and spin-photon behavior. Utilizing scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM), this study visually depicts the disruption of symmetry in two typical atomic quantum emitters within MoS_2 layers. By changing the substrate chemical potential, a variety of charge states for sulfur vacancies (Vac_S) and substitutional rhenium dopants (Re_{Mo}) are stabilized. Vac_S^{-1}, Re_{Mo}^{0} and Re_{Me}^{-1} exhibit distinct local lattice distortions and symmetry-broken defect orbitals, attributed to Jahn-Teller effect (JTE) and *pseudo*-JTE. This research disentangles the impact of spatial averaging, charge multistability, configurational dynamics and external perturbations through atomic-scale mapping of electronic and geometric structures.

Authors' comments:
"Using atomically-resolved scanning probe microcopy we unveil how the charge state of single defects correlates with the local lattice symmetry, affecting their functionality in 2D semiconductors. This understanding is critical for their applications in nanoelectronics and quantum photonics."



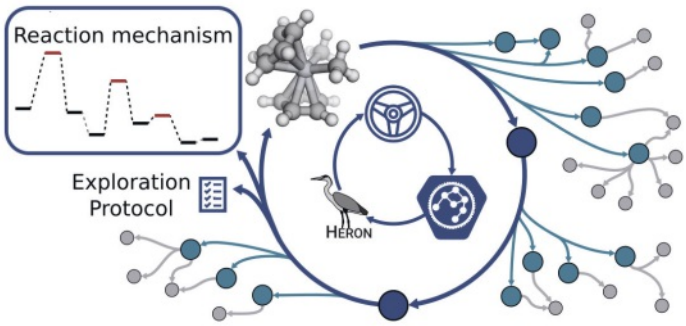
A Human-machine Interface for Automatic Exploration of Chemical Reaction Networks

Miguel Steiner, Markus Reiher

Nat. Commun. **2024**, *15*, 3680
https://doi.org/10.1038/s41467-024-47997-9
ETH Zurich

This article describes the STEERING WHEEL algorithm, offering a guided approach to exploring complex chemical processes. It addresses the limitations of brute-force autonomous quantum-chemical methods and rigid constraints, enabling focused investigation of specific regions within vast reaction networks. Particularly beneficial for elucidating reaction mechanisms in transition metal catalysis, this intuitive and adjustable method aids in both structure-specific calculations and broad high-throughput screening of potential intermediates. By guiding automated data generation, it facilitates reproducible exploration and optimization in chemistry, promising insights into intricate processes and aiding advancements in catalyst design and mechanism elucidation.

Authors' comments:
"Automated quantum chemistry delivers unprecedented details of reaction mechanisms, at the cost of an enormous amount of computations. To tame this by human insights, the STEERING WHEEL allows one to control an otherwise autonomous exploration in an intuitive way."



Prepared by Cesare Berton, Patrick A. Cieslik, Simon Klinger, Jonas Genz, Eda Nisli, Fan Liu, Stanislav Prytuliak, Deborah Bäcker, Perle Hermant, Samy Kichou, Ben Boback, 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

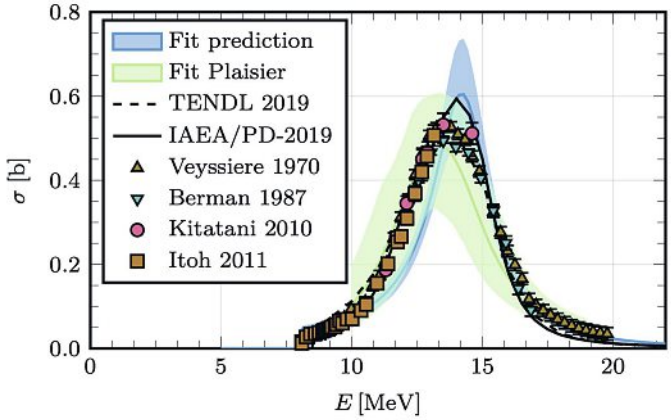
Methodology for Measuring Photonuclear Reaction Cross Sections with an Electron Accelerator Based on Bayesian Analysis

Saverio Braccini, Pierluigi Casolaro, Gaia Dellepiane, Christian Kottler, Matthias Lüthi*, Lorenzo Mercolli, Peter Peier, Paola Scampoli, and Andreas Türler

App. Radiat. Isot. **2024**, *208*, 111275
https://doi.org/10.1016/j.apradiso.2024.111275
University of Bern, Federal Institute of Metrology (METAS)

Accurate measurements of photonuclear reaction cross sections are essential for various applications, such as radiation shielding design, absorbed dose calculations, reactor physics, nuclear safeguard, astrophysics, and nuclear medicine. To address the production of specific radionuclides like ^{225}Ac, ^{47}Sc, and ^{67}Cu, the authors developed a methodology utilizing the microtron accelerator at the Swiss Federal Institute of Metrology (METAS). This approach involves measuring the produced activity using a High Purity Germanium (HPGe) gamma spectrometer and employing Monte Carlo simulations to determine the photon fluence spectrum. Data analysis employed a Bayesian fitting procedure on experimental data, assuming a Breit-Wigner model for the cross-section. Validation of this methodology was conducted by measuring the well-established photonuclear cross-section of the ^{197}Au(γ, n)^{196}Au reaction, yielding results consistent with existing literature.

Authors' comments:
"We have developed and verified a straightforward approach to measure photonuclear cross-sections. The graph below shows the measured ^{197}Au(γ, n)^{196}Au cross-section in comparison with earlier measurements and evaluated data."



RNA Oligomers at Atomic Resolution Containing 1-Methylpseudouridine, an Essential Building Block of mRNA Vaccines

Philipp Nievergelt, Florian Berliat, Katherine E. McAuley, Colin R. Dorgan, Renate Maria van Well, Andrea Thorn, and Bernhard Spingler*

Chem. Med. Chem. **2024**, *19*
https://doi.org/10.1002/cmdc.202300600
University of Zurich

The study focused on elucidating the structural characteristics of 1-methylpseudouridine (m1Ψ), both independently and within the context of double-stranded RNA structures. By employing high-resolution crystallography techniques, the research successfully determined the first detailed structures of RNA oligomers containing m1Ψ. These findings not only shed light on the structural similarities between m1Ψ-modified RNA and its native counterpart but also revealed its isostructural relationship with 5-methyluridine (m5U) in the crystalline state. Additionally, the study expanded upon previous investigations by examining the melting temperatures of short, modified RNA oligos, contributing further insights into the thermodynamic stability of m1Ψ-modified RNA. Overall, this work advances the understanding of the structural and functional implications of m1Ψ in RNA biology, with potential implications for therapeutic and biotechnological applications.

Authors' comments:
"Complete substitution of uridine by m1Ψ was found to be essential for the success of the mRNA vaccines. We were pleased to achieve crystal structures with true atomic resolution (up to 1.01 Å) of m1Ψ modified RNA oligomers. This was done by solving one structure *ab initio* without any further input."