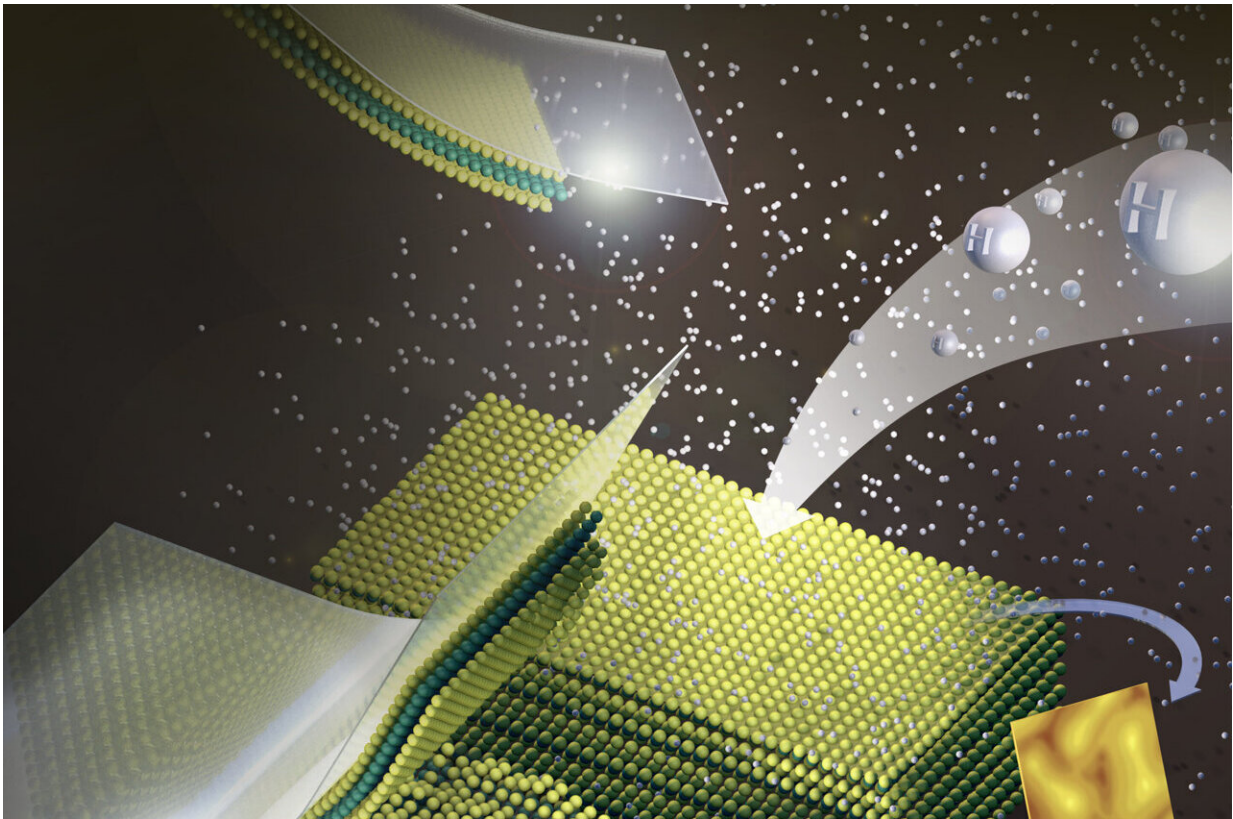


Neutralizing electronic inhomogeneity in cleaved bulk MoS₂

November 1 2023, by Sonal Mistry



The illustration shows the MoS₂ lattice structure (green: Mo, yellow: S). The material after cleaving is shown in the forefront, the surface is jagged, and the measured surface electronic structure is inhomogeneous (colored map). In the back is the cleaved material after exposure to atomic hydrogen (represented by the white balls). The measured surface electronic structure, shown in the map, is more homogenous. Credit: Martin Küsting / HZB

Molybdenum disulfide (MoS_2) is a highly versatile material that can function, for example, as a gas sensor or as a photocatalyst in green hydrogen production. Although the understanding of a material usually starts from investigating its bulk crystalline form, for MoS_2 much more studies have been devoted to mono and few layer nanosheets.

The few studies conducted thus far show diverse and irreproducible results for the electronic properties of cleaved bulk MoS_2 surfaces, highlighting the need for a more systematic study.

Dr. Erika Giangrisostomi and her team at HZB carried out such a systematic study at the LowDosePES end-station of the BESSY II light source. They utilized X-ray photoelectron spectroscopy technique to map the core-level electron energies across extensive surface areas of MoS_2 samples. Using this method, they were able to monitor the changes in the surface [electronic properties](#) after in-situ ultra-high-vacuum cleaving, annealing and exposure to atomic and [molecular hydrogen](#).

The results from this study point to two main findings. Firstly, the study unambiguously reveals sizeable variations and instabilities in electron energies for the freshly cleaved surfaces, demonstrating how easy it is to come to diverse and irreproducible outcomes. Secondly, the study shows that [room temperature](#) atomic [hydrogen](#) treatment is remarkably effective in neutralizing the [surface](#) electronic inhomogeneity and instability.

This is rationalized by the ability of hydrogen atoms to either accept or give away an electron, and calls for further characterizations of the functional properties of the hydrogenated material. "We hypothesize that atomic hydrogen helps rearranging sulfur vacancies and excess of sulfur atoms yielding a more ordered structure," Erika Giangrisostomi says.

This study marks a fundamental step in the investigation of MoS_2 . Due

to the extensive use of MoS₂ in all kinds of applications, the findings of this research have the potential to reach a wide audience in the fields of electronics, photonics, sensors and catalysis.

The study is [published](#) in the journal *Advanced Materials Interfaces*.

More information: Erika Giangrisostomi et al, Inhomogeneity of Cleaved Bulk MoS₂ and Compensation of Its Charge Imbalances by Room-Temperature Hydrogen Treatment, *Advanced Materials Interfaces* (2023). [DOI: 10.1002/admi.202300392](https://doi.org/10.1002/admi.202300392)

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