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Preference: ORAL presentation (*invited*)

Exploring the Flatland of 2D materials by electrochemical STM: visualization of the active sites for the hydrogen evolution reaction with atomic scale precision

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2D materials such as chemically modified graphenes, transition metal dichalcogenides, layered double hydroxide to name only a few, are having a huge impact on electrocatalysis providing materials with outstanding activity for a variety of reactions.[1]

However, despite the intense research efforts in this field, a clear identification of the real active sites in many reactions remains a great challenge, given the necessity to employ *spatially and structurally sensitive techniques* in *operando* conditions (i.e. during the application of an electrochemical potential in the presence of an electrolyte).

Here we present an innovative approach to the study of 2D materials by using electrochemical Scanning tunneling microscopy. As demonstrated by a seminal paper,[2] this technique allows identifying the presence of catalytic processes *at the nanoscale* by observing a typical noise in the tunneling current, which is due to instantaneous variations of the tunneling junction.

By using special model systems consisting of CVD grown transition metal dichalcogenides thin films (MoSe₂ and WSe₂), and iron ultrathin films covered by graphene, we achieved even *atomic resolution in operando* during the hydrogen evolution reactions. This allowed us to distinguish the chemical activity of several chemical and morphological features such as single atom vacancies, Fe-C₄ defects, step edges, and even exotic line defects such as metallic twin boundaries.[3]

References

- [1] Chia, X., Pumera, M. *Nature Catalysis* **2018**, *10*, 909-921
- [2] Pfisterer, J.H., Liang, Y., Schneider, O. Bandarenka, A.S., *Nature*, **2017**, *549*, 74.
- [3] Kosmala, T., H. Coy-Diaz, Komsa, H.-P., Ma. Y., Krasheninnikov, A., Batzill, M. Agnoli S. *Advanced Energy Materials* **2018** 180031

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