# Identifying and Probing Atomic Defects in 2D Semiconductors by Scanning Probe Microscopy

L. Huberich[1] J. Allerbeck[1] L. Bobzien[1] E. Ammerman[1] O. Gröning[1] R. Hennig[2] D. Qiu[3] J. Robinson[4] B. Schuler[1]

[1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland
[2]Department of Materials Science and Engineering, University of Florida, USA
[3]Department of Mechanical Engineering and Materials Science, Yale University, USA
[4]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA

Two-dimensional (2D) semiconductors provide an exciting platform to engineer atomic quantum systems in a robust, yet tunable solid-state system. In this talk, I will present our efforts to un-ravel the interesting physics behind single vacancies and dopant atoms in transition metal dichal-cogenide (TMD) mono- and multilayers by means of high-resolution scanning probe microscopy [1-6]. I will highlight how to generate atomic defects by different means, and how to identify them based on their characteristic scanning tunneling spectroscopy (STS) fingerprint and density functional theory modelling. Our recent studies on transition metal doped TMDs such as (n-type) Re-doped $MoS_2$ and (p-type) V-doped $WSe_2$ reveals the significance of the charge state in the spectroscopic signa-ture of these defects. By substrate chemical gating, we can stabilize three charge states of $Re_{Mo}$, where two of the charge states exhibit symmetry broken electronic orbitals and a distorted atomic configuration that we assign to a pseudo Jahn-Teller effect [7]. Negatively charged V dopants and dopant pairs in $WSe_2$ exhibit a series of occupied p-type defect states above the va-lence band edge, accompanied by an intriguing electronic fine-structure that we attribute to many-body electron interactions [8].Lastly, I will provide an outlook on our ongoing developments of ultrafast lightwave-driven scanning tunneling microscopy using single-cycle THz pulses to measure the sub-picosecond time dynamics at atomic spatial resolution [9].

[1] B. Schuler et al., *Phys. Rev. Lett.* **123**, 076801 (2019).
[2] B. Schuler et al., *ACS Nano* **12**, 10520 (2019).
[3] S. Barja et al., *Nat. Commun.* **10**, 3382 (2019).
[4] B. Schuler et al., *Sci. Adv.* **6**, eabb5988 (2020).
[5] K. Cochrane et al., *Nat. Commun.* **12**, 7287 (2021).
[6] E. Mitterreiter et al., *Nat. Commun.* **12**, 3822 (2021).
[7] F. Xiang*, L. Huberich* et al., *Nat. Commun.* , (2024).
[8] S. Stolz et al., *ACS Nano* **17**, 23422 (2024).
[9] J. Allerbeck et al., *ACS Photonics* **10**, 3888 (2023).