Two-dimensional transition-metal dichalcogenides with tailored properties

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Layered transition-metal dichalcogenides have shown the potential to achieve two-dimensional (2D) materials, similar to the exfoliation of graphene from graphite. Using first-principles calculations, we study prototypical monolayer MoS2 to obtain insight into the influence of defects and substitutional doping on the material properties, for a wide range of transition-metal dopants. We also address polar transition-metal dichalcogenide monolayers with respect to both their structural stability and the consequences of the strong spin-orbit coupling. Finally, heterojunctions of MoS2 with unsaturated and saturated MXenes are discussed. These hyrid systems are interesting for application in all-2D devices.

Short Bio:
Udo Schwingenschlogl is a Professor in the Physical Sciences and Engineering Division of King Abdullah University of Science and Technology (KAUST). Before joining KAUST in September 2008, he has worked at the International Center of Condensed Matter Physics in Brasilia, Brazil, and the University of Augsburg in Germany.