Ab-initio Discovery and Characterization of Novel 2D Materials for Energy Technologies and Electronic Devices.

Abstract: The rapid rise of novel 2D materials, presents the exciting opportunity for materials science to explore an entirely new class of materials. This comes at the time when mature computational methods provide the predictive capability to enable the computational discovery, characterization, and design of 2D materials and provide the needed input and guidance to experimental studies. I will present our high-throughput, data-mining, and evolutionary algorithm approaches to identify novel 2D materials with low formation energies and show how unexpected structures emerge when a material is reduced to sub-nanometers in thickness. We discovered several 2D materials in the families of group III-V compounds and group-II oxides with promising properties for electronic devices and identify suitable metal substrates that can stabilize several of these as-yet hypothetical materials. In the families of group-III monochalcogenides and transition metal dichalcogenides we identify several 2D materials that are suitable for photocatalytic water splitting. For several transition-metal chalcogenide compounds we find that ferromagnetic order emerges at temperatures accessible to experiments. This opens the opportunity to investigate the interplay of magnetic order and reduced dimensionality and may provide materials for spintronics applications. Our results provide guidance for experimental synthesis efforts and future searches of materials suitable for applications in energy technologies and electronic devices.

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Professor Hennig received his Diploma in Physics at the University of Göttingen in 1997 and his Ph.D. in Physics from Washington University in St. Louis in 2000. After working as a postdoctoral researcher and research scientist at Ohio State University, he joined the faculty of the Department of Materials Science and Engineering at Cornell in 2006 as an Assistant Professor. In 2014 he moved to the University of Florida as an Associate Professor. His research focuses on the development and application of computational methods for 2D materials and interfaces.