

Chemistry and Physics of 2D heterostructures

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Biography

Thomas Heine, FRSC, MAE (PhD 1999, *venia legendi* 2006 TU Dresden) started his research group in 2008 at Jacobs University Bremen, moved in 2015 to University of Leipzig and 2018 to his current position as chair professor of theoretical chemistry at TU Dresden. He is a Clarivate Highly Cited Researcher with more than 420 peer-reviewed articles, an h-index of 98 (ISI) / 110 (Google Scholar), and more than 43000 citations. Prof. Heine is elected member of the Review Board of Deutsche Forschungsgemeinschaft (DFG). He coordinates DFG Priority Program PP 2244 “2D Materials: Physics of van der Waals [hetero]structures”, the DFG Researcher Training Group RTG 2861 “Planar Carbon Lattices”. He holds a prestigious ERC Synergy Grant (2DPolyMembrane) and a DFG Reinhart-Koselleck project (top funding scheme for individuals by DFG). His current research interests focus on magnetic metal-free materials and of precision membranes for selective unidirectional ion transport.

Abstract

One of the most fascinating effects of two-dimensional (2D) crystals is the proximity effect, which, for example, changes the band character in transition metal dichalcogenides. While density-functional theory (DFT), the working horse computational method in the field, correctly describes the impact of the proximity effect on the electronic structure, the prediction of interlayer distances is less straight-forward. This is an issue if the interlayer interaction can result in different isomeric structures, sometimes with strongly different electronic characteristics, such as in blue phosphorene, gray arsenene or its bilayers. As a side note, even the nomenclature of the stacking symmetry is not straight-forward. Twisted bilayers are known to form moiré structures which can further relax to stacking domains separated by superlattices, where the latter ones dominate the electronic structure near the fermi level. The emergence of 2D crystals with magnetic ordering has called for the investigation of the interlayer magnetic interactions. Intriguingly, one can transfer magnetic moments inbetween layers by optical excitations as revealed by real-time time-dependent DFT calculations. We have recently extended our efforts to couple organic 2D crystals, which are made of organic molecules that are stitched together with strong bonds to form a regular crystal with the traditional 2D crystals. Also organic 2D crystals are subject to a strong proximity effect, and strong couplings are observed in their heterostructures with graphene.