



## PHYSIKALISCHES KOLLOQUIUM

*Referent:* **Prof. Dr. Thomas Heine**  
Chair of Theoretical Chemistry,  
TU Dresden, Germany



*Thema:* **A computational approach towards new physics in 2D materials**

*Zeit und Ort:* Dienstag, 9.4.2019, 16:40 Uhr  
Recknagel-Bau, Hörsaal REC/C213, Haeckelstr. 3

*Leiter:* Prof. Dr. Matthias Vojta

*Kurzfassung:* The discovery of graphene initiated an immense research effort in the field of two-dimensional (2D) crystals. Soon it was clear that 2D crystals can be formed from virtually all layered materials by top-down, but also bottom-up approaches. The family of 2D materials contains a lot of remarkable phenomena. It is somewhat less known that graphene represents also the prototype 2D polymer. 2D polymers (also 2D covalent-organic frameworks – 2D COFs) are a rather new family of synthetic 2D crystals where molecular units are stitched together with strong bonds. This offers a regular crystal lattice and thus materials comprising all collective phenomena that are known from solid state physics. A recent breakthrough was the discovery of chemical coupling reactions that achieve full conjugation between the constituting molecules, which is the precondition for the formation of 2D semiconductors with ballistic transport properties. For the 2D polymers I will to focus on structural diversity: while mathematically, 11 tilings are possible in two-dimensions (the so-called Kepler nets), nature offers much less structural diversity in crystalline 2D materials. By picking suitable molecular building units we can form lattices with structural topologies that impose, in turn, electronic topologies. One of the examples that I will highlight is the kagome structure, which produces both Dirac points and flat bands.

*Biographie:* Prof. Heine is Full Professor of Theoretical Chemistry at TU Dresden and Adjunct Professor of Theoretical Physics at Jacobs University Bremen, Germany. In 1995 he received his diploma (physics) at TU Clausthal, Germany, and in 1999 his PhD (physics) at TU Dresden. After postdoctoral stages, he started his research group in 2008 as Associate Professor at Jacobs University Bremen, where he was promoted to Full Professor in 2011. From 2015-2018 he held the Chair of Theoretical Chemistry at Leipzig University, and in 2018 he accepted the offer for the Chair of Theoretical Chemistry associated with a group leader position a Helmholtz Center Dresden-Rossendorf. His research interest is the computational science of nanostructured materials, in particular of two-dimensional crystals and molecular frameworks.

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