

## Theoretical Chemistry Colloquium

# October 3, 2014 (Fri), 15:00-16:00

## RCMS, 2<sup>nd</sup> floor, Chemistry Gallery

### *Transition metal dichalcogenides: a highly sensitive species*

**Prof. Thomas Heine**

School of Engineering and Science  
Jacobs University, Bremen, Germany



**Abstract:** Transition metal dichalcogenides have been shown to exhibit extraordinary mechanical, chemical and electronic properties, leading to applications in catalysis, lubrication and nanoelectronics. They are also known to be able to strongly alter their properties due to the intriguing electronic interplay of the transition metal as well as on the delicate electronic structure, strongly influenced by the electronic system that is formed in the transition metal layer. The electronic properties of transition metal dichalcogenides change by the number of layers, by strain, by exposing them to external fields, by the type of defects.

In my presentation I address the situations where transition metal dichalcogenides are particularly sensitive, and will provide the rationale for it, as understanding those phenomena are crucial for the rational design of devices based on these species. I will further give an outlook at noble metal dichalcogenides. A large part of the content that will be covered is published in the contributions below.

#### **References:**

- *An Atlas of Two-Dimensional Materials.* P. Miro, M. Audiffred, T. Heine, *Chem. Soc. Rev.* (2014), DOI: 10.1039/c4cs00102h.
- *Electron Transport in MoWSeS Monolayers in Presence of an External Electric Field.* N. Zibouche, P. Philippsen, T. Heine, A. Kuc, *Phys. Chem. Chem. Phys.* 16 (2014) 11251-11255.
- *Two Dimensional Materials Beyond MoS<sub>2</sub>: Noble Transition Metal Dichalcogenides.* P. Miro, M. Ghorbani-Asl, T. Heine, *Angew. Chem. Intl. Ed. Engl.* 53 (2014) 3015–3018.
- *Defect-induced conductivity anisotropy in MoS<sub>2</sub> monolayers.* M. Ghorbani-Asl, A. N. Enyashin, A. Kuc, G. Seifert, T. Heine, *Phys. Rev. B* 88 (2013) 245440.
- *Electromechanics in MoS<sub>2</sub> and WS<sub>2</sub>: nanotubes vs. monolayers.* M. Ghorbani-Asl, N. Zibouche, M. Wahiduzzaman, A. F. Oliveira, A. Kuc, T. Heine, *Scientific Reports* 3 (2013) 2961.
- *Spontaneous Ripple Formation in MoS<sub>2</sub> Monolayers: Electronic Structure and Transport Effects.* P. Miro, M. Ghorbani-Asl, T. Heine, *Adv. Materials* 25 (2013) 5473–5475.

#### **Contact:**

Stephan Irle, 6397, sirle@chem.nagoya-u.ac.jp

