



Institute for Materials Science
Universität Stuttgart

Colloquium
Materials Science
Summer Semester 2020

Joint colloquium with
Institute of Organic Chemistry

Tuesday 23 June 2020 @ 5:15pm

On-line per WebEx !

Meeting number: 121 109 9421

Meeting password: sUmJARU5X34

Meeting link:

<https://kurzelinks.de/mawikolloquium-ss20-atkatchenko>

"Accurate and Efficient Models for Covalent and Non-Covalent Interactions in Molecules and Materials"

Prof. Dr. Alexandre Tkatchenko

Theoretical Condensed Matter Physics, University of Luxembourg

Abstract: This talk will concern the development of efficient, yet potentially very accurate, models to describe covalent and non-covalent (van der Waals) interactions in molecules and materials. For local chemical interactions, we have developed symmetric force-based machine learning techniques that allow to achieve the "gold standard" quantum-chemical accuracy in the description of potential-energy surfaces of molecules and solids [1,2]. For non-covalent interactions, we have developed coarse-grained quantum-mechanical models for interatomic potentials based on coupled harmonic oscillators [3,4]. The accuracy, efficiency, and insight that can be obtained from both approaches will be demonstrated on the example of molecular spectroscopy [2], polymorphism in molecular crystals [5], and plasmon-like fluctuations in solvated proteins [6]. All our developments are firmly motivated by challenging experimental observations, and I make connections to experiments throughout the talk.

- [1] S. Chmiela et al., *Science Adv.* 3, 1603015 (2017).
- [2] S. Chmiela, H. E. Sauceda, K. R. Mueller, and A. Tkatchenko, *Nature Commun.* 9, 3887 (2018).
- [3] J. Hermann, R. A. DiStasio Jr., and A. Tkatchenko, *Chem. Rev.* 117, 4714 (2017).
- [4] M. Stoehr, T. Van Voorhis, and A. Tkatchenko, *Chem. Soc. Rev.* 48, 4118 (2019).
- [5] J. Hoja et al., *Science Adv.* 5, eaau3338 (2019).
- [6] M. Stoehr and A. Tkatchenko, *Science Adv.* 5, eaax0024 (2019).

Host: Prof. Dr. Clemens Richert
Prof. Dr. Blazej Grabowski

