

## Theoretical Chemistry Colloquia (SS 2018)

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Time: wednesdays 14:15, Location: Seminarraum NC 03/399

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25. 04. 2018      **Sebastian Stolzenberg**, Computational Molecular Biology, Freie Universität Berlin  
*Mechanistic Insights into MHC class II proteins using Molecular Dynamics Simulations and Markov State Modeling*  
 (Joint seminar with EXC 1069 "RESOLV")
16. 05. 2018      **Ulrich Kleinekathöfer**, Department of Physics and Earth Sciences, Jacobs University Bremen gGmbH  
*Transport across Bacterial Membranes: Insights from Molecular Simulations*  
 (Joint seminar with EXC 1069 "RESOLV")
30. 05. 2018      **Karin Fink**, Karlsruher Institut für Technologie (KIT), Institut für Nanotechnologie, Karlsruhe  
*Ab initio calculations for transition metal chemistry*
06. 06. 2018      **Mario Barbatti**, Institut de Chimie Radicalaire, Aix-Marseille Université, Marseille, France  
*Nonadiabatic mixed quantum-classical dynamics simulations applied to organic molecules and assemblies*
13. 06. 2018      **Andreas Köhn**, Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart  
*Accurate methods for complicated electronic structures*
20. 06. 2018      **Manuel Hochheim**, Mulliken Center for Theoretical Chemistry, Universität Bonn  
*Surface Band-edge Levels From Current Hybrid DFT Methods, and Their Applications*  
 (Speaker Exchange Program Bonn/Bochum)
27. 06. 2018      **Sebastian Höfener**, Karlsruher Institute of Technology (KIT), Institute of Physical Chemistry, Karlsruhe  
*Computing molecular properties in complex environments using frozen-density embedding methods*  
 (Joint seminar with EXC 1069 "RESOLV")
04. 07. 2018      **Holger Gohlke**, Computational Pharmaceutical Chemistry, Heinrich-Heine-University, Düsseldorf  
*Rigidity theory-based perturbation approach to analyze dynamic allostery*  
 (Joint seminar with EXC 1069 "RESOLV")
11. 07. 2018      **Alexander Auer**, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr  
*From old methods for new applications to new methods for old problems - DFT for electrochemistry and tensor decomposition FCI*

gez. Die Dozenten der Theoretischen Chemie

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