

Einladung zum Mini-Symposium
Current developments in vibrational structure theory
des Ortsverbandes Hannover 2023

am Montag, 19.06.2023
im kleinen Hörsaal der anorganischen Chemie
(Raum 101, Gebäude 2501), Callinstr. 3-9, 30161 Hannover

- 14:00 Welcome (C. König)
- 14:05 Kiyoshi Yagi (RIKEN, Saitama, Japan)
*Anharmonic vibrational calculations of complex systems:
Applications to biomolecules and polymer materials*
- 14:45 Janine Hellmers (Leibniz Universität Hannover) *Tailored
vibrational structure theory for spectroscopic signatures*
- Christoph Jacob (TU Braunschweig)
- 15:15 *Anharmonic theoretical vibrational spectroscopy with
localized modes*
- 15:45 – 16:15 Pause**
- 16:15 Guntram Rauhut (Universität Stuttgart)
*Accurate VCI calculations as a prerequisite for reliable
rovibrational spectra*
- 16:55 Julia Brüggemann (TU Braunschweig)
Quantum-chemical calculations of 2D-IR spectra
- 17:25 Benjamin Schröder (Georg-August-Universität Göttingen)
Incremental vibrational configuration interaction theory (iVCI)
- 17:55 Closing (C. König)
- 18:30 Nachsitzung**