Poster Slam – Session A

P7	Ehrmaier, J.; Domcke, W.; Sobolewski, A. L.	A Theoretically Conceived Photochemical Pathway to Solar Water Splitting Using Carbon Nitride Chromophores
P11	Goerigk, L.	What We can Learn from Comprehensive Benchmark Studies: Insights for Method Developers and Users
P15	Schran, C.; Behler, J.; Marx, D.	Neural Network Potentials for Solvation: Protonated Water Clusters in Superfluid Helium
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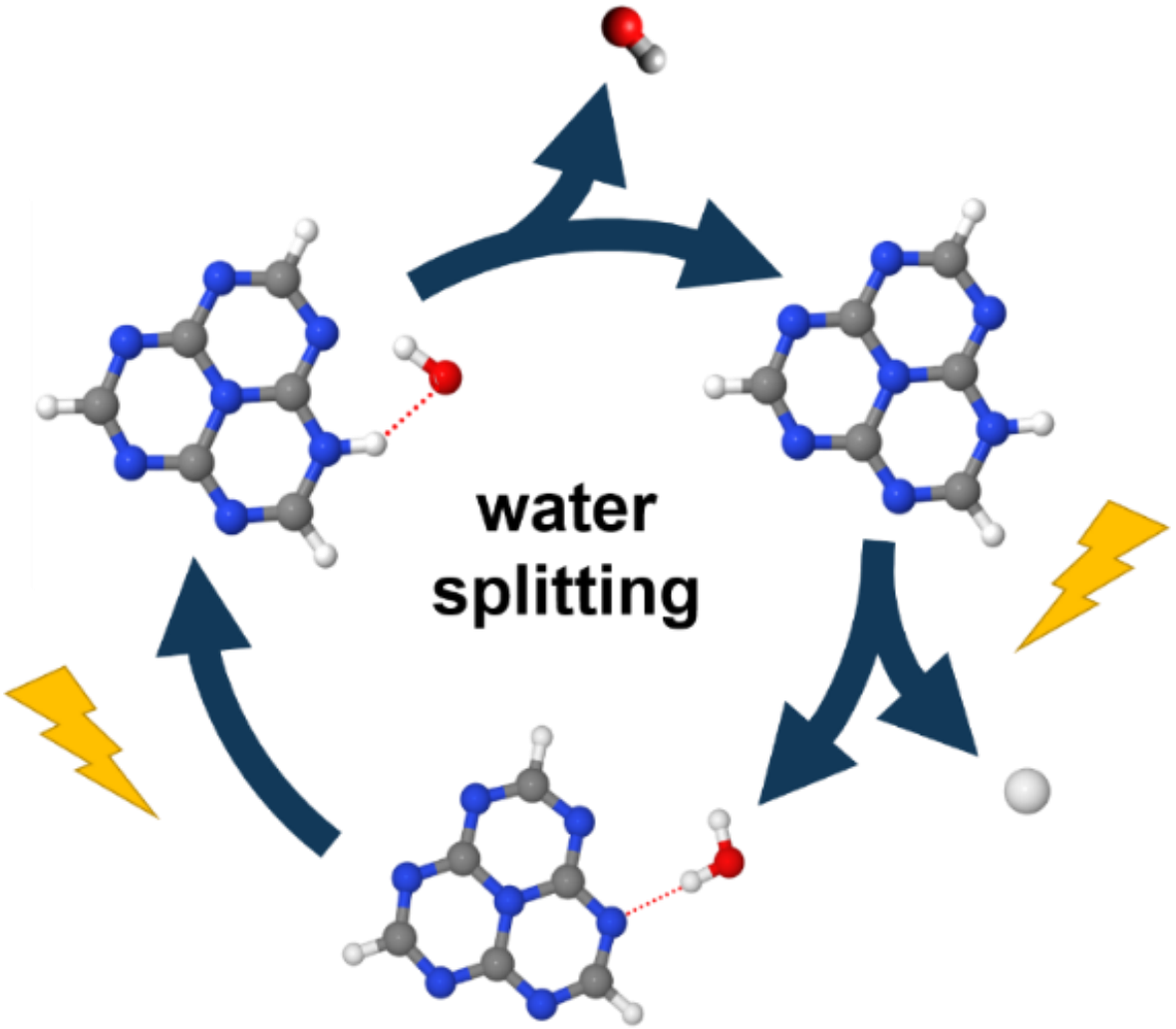
P007



Johannes Ehrmaier

Poster Slam – Session A

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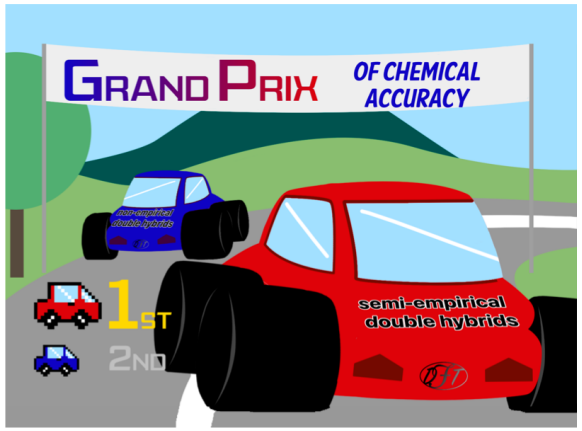
Poster P011: The largest DFT benchmark study

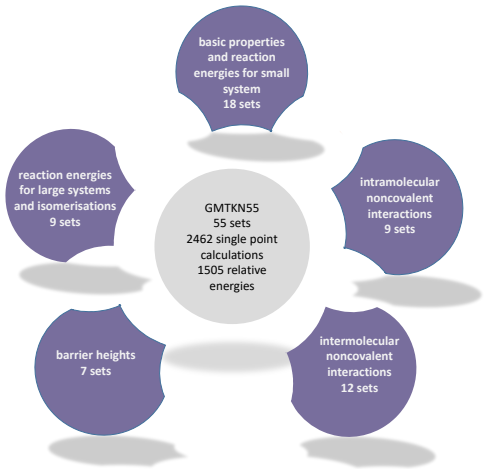
- **325 dispersion-corrected and –uncorrected methods**
- Getting rid of **misconceptions** around:
  - van-der-Waals functionals[1]
  - non-empirical double-hybrid functionals[2]
  - which functionals to use/avoid (for users)[1,2,3]
- special **challenge** for method developers

[1] Najibi, Goerigk, *PCCP* **2018**, manuscript submitted to JCTC.
[2] Mehta, Casanova-Páez, Goerigk, *PCCP* **2018**, DOI: 10.1039/C8CP03852J.
[3] Goerigk, Hansen, Bauer, Ehrlich, Najibi, Grimme, *PCCP* **2017**, *19*, 32184. (***Open Access***)

2017 "Hot Article"[3]



2018 "Hot Article"[2]



THE UNIVERSITY OF MELBOURNE

Melbourne Centre for Theoretical and Computational Chemistry

Poster Slam – Session A

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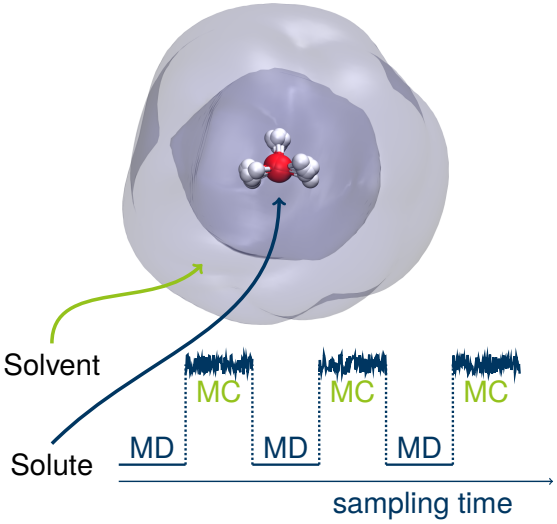
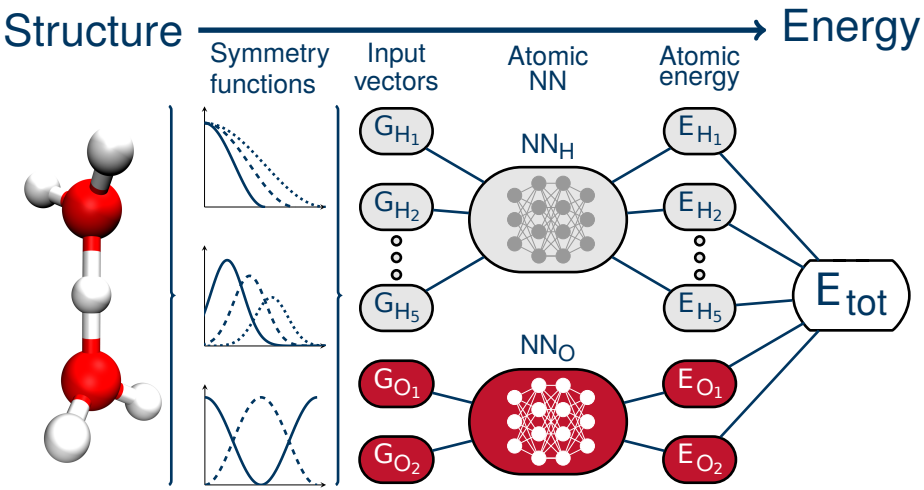
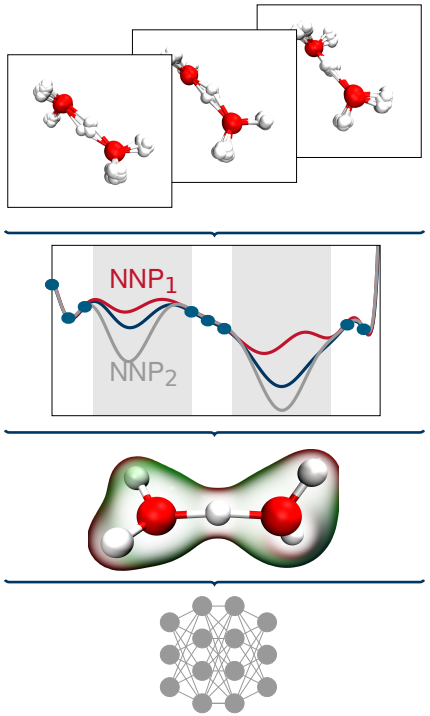
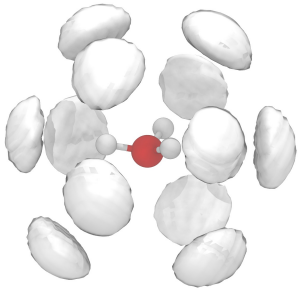
Neural Network Potentials for Solvation: Protonated Water Clusters in Superfluid Helium

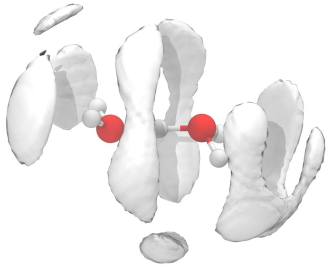


High–Dimensional Neural Network Potentials









Poster #15

C. Schran, F. Uhl, J. Behler, D. Marx, J. Chem. Phys. **2018** 148, 102310.

RUB

RESOLV
RUHR EXPLORES SOLVATION
CLUSTER OF EXCELLENCE - EXC 1069

Christoph Schran and Dominik Marx
Lehrstuhl für Theoretische Chemie
Ruhr–Universität Bochum, 44780 Bochum, Germany
christoph.schran@rub.de

Poster Slam – Session A

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Dispersion Corrections from First Principles and Machine Learning

Jonny Proppe, Stefan Gugler, Markus Reiher | ETH Zürich

We already quantified statistical errors in dispersion corrections → Talk by Thomas Weymuth (C26)

What about systematic errors? → Gaussian process (GP) regression

$$f_*^{\mathrm{D3}}\left(C_6R^{-6}\right) \xrightarrow{\mathcal{GP}\left(\left\{f_i^{\mathrm{D3}}\left(C_6R^{-6}\right),\Delta E_{\mathrm{disp},i}^{\mathrm{QM}}\right\}\right)} \Delta E_{\mathrm{disp},*}^{\mathrm{GP}} \sim \mathcal{N}\left(\mu_{*,\{i\}},\sigma_{*,\{i\}}^2\right)$$

A) CORRECTS FOR SYSTEMATIC ERRORS, B) PROVIDES RELIABLE ERROR BARS, C) BASED ON D3-TYPE INTERACTIONS ONLY

Poster Slam – Session A

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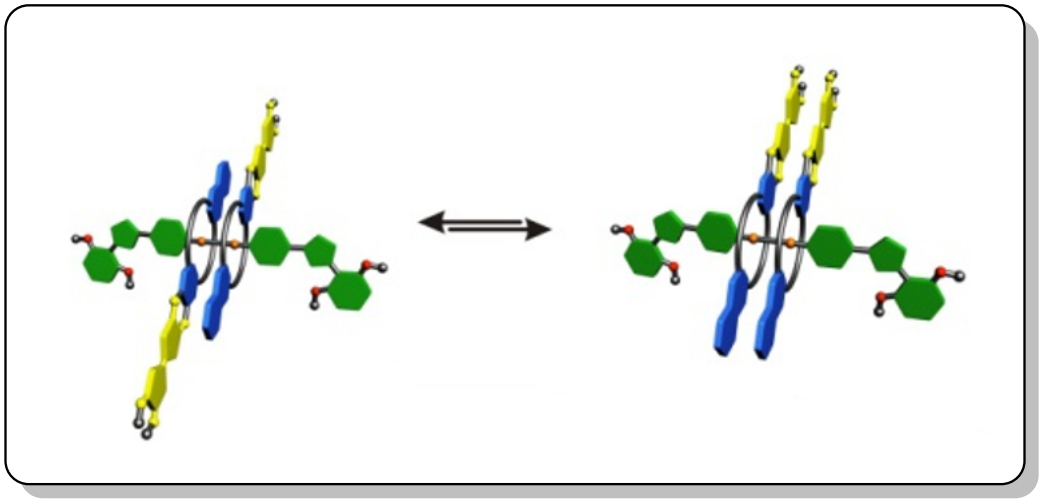
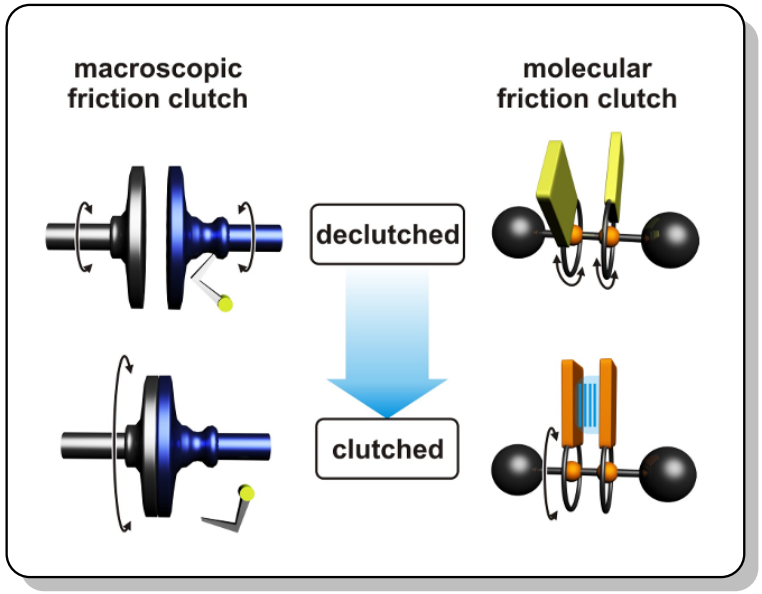
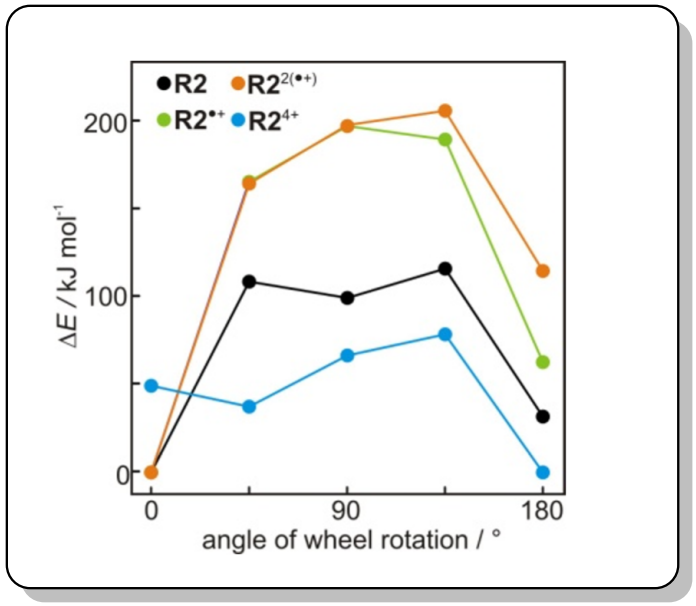
Non-covalent interactions in supramolecular frameworks:

When experiment does not suffice (P049)







H. V. Schröder, F. Witte, M. Gaedke, S. Sobottka, L. Suntrup, H. Hupatz, A. Valkonen, B. Paulus, K. Rissanen, B. Sarkar, C. A. Schalley, *Org. Biomol. Chem.* **2018**, 16, 2741.; H. V. Schröder, A. Mekic, H. Hupatz, S. Sobottka, F. Witte, L. Urner, M. Gaedke, K. Pagel, B. Sarkar, B. Paulus, C. A. Schalley, *submitted*.

Poster Slam – Session A

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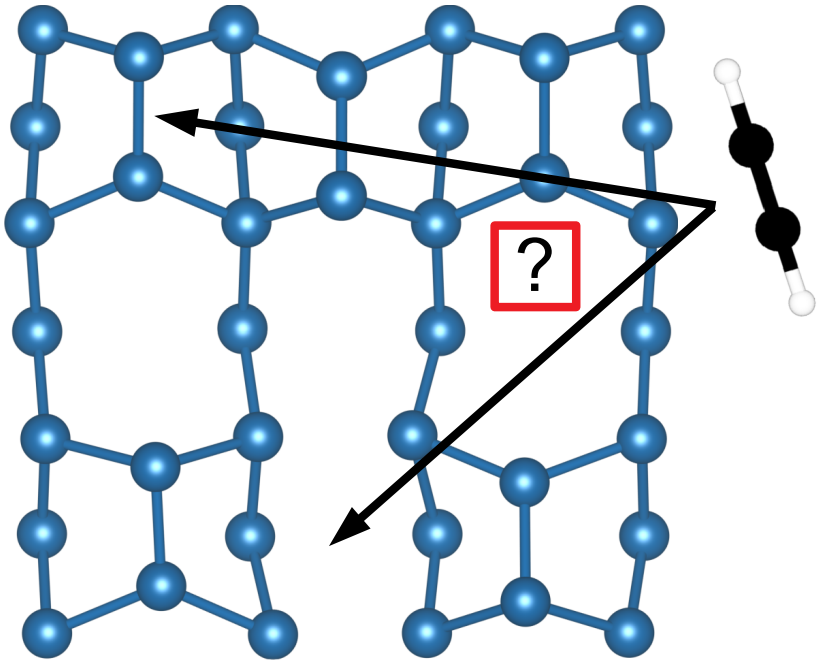
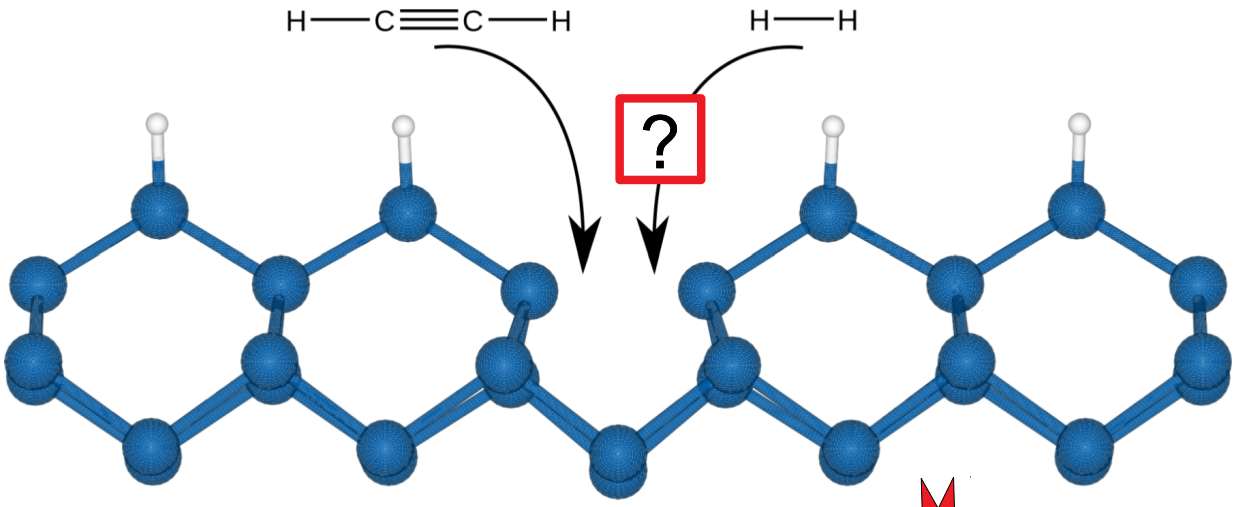
Si(001) defects and their impact on surface reactivity



Is there a seed for selective adsorption?



Is the surface more reactive?

SFB 1083
Structure and Dynamics of Internal Interfaces

> Tonner.group

J.-N. Luy

Poster: P055

Poster Slam – Session A

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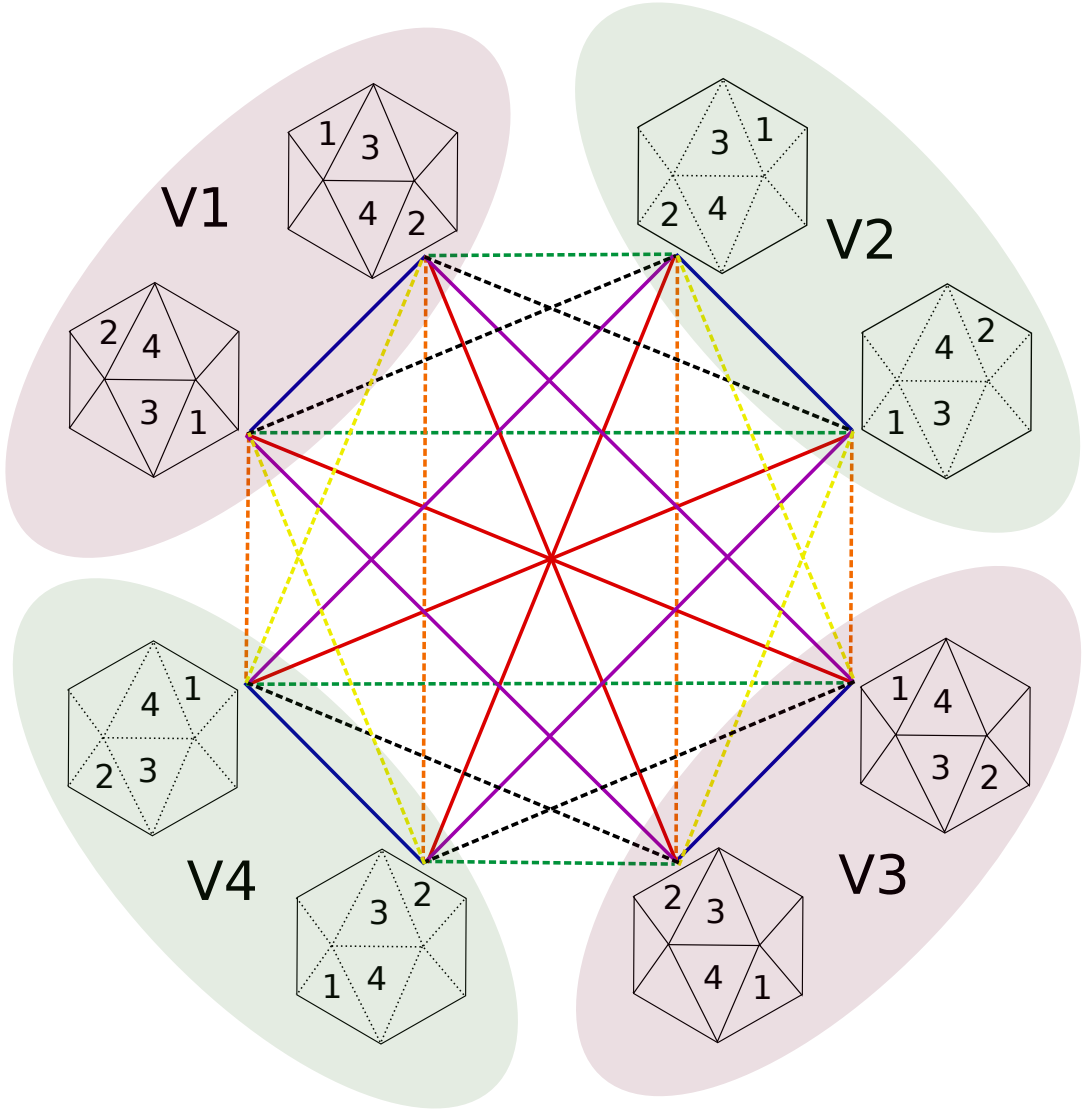
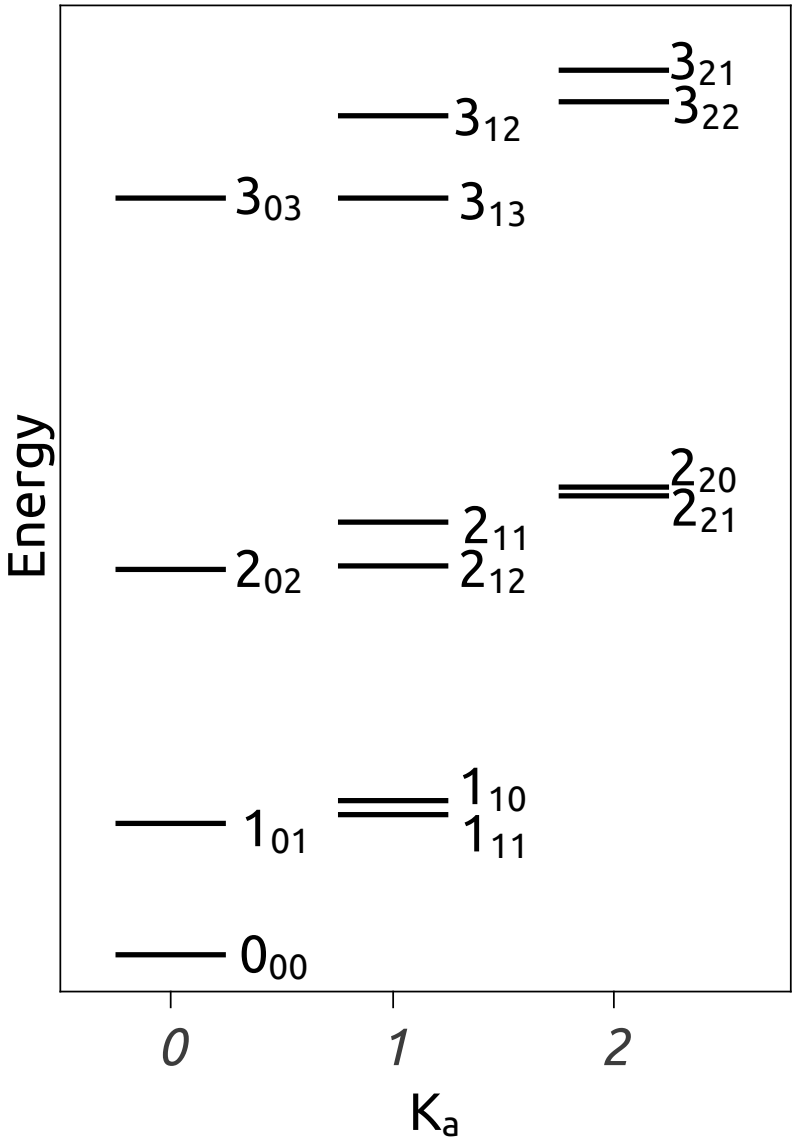
P071: Rotational Spectra of Chiral Systems

Tunneling splitting in chiral clusters using the molecular symmetry group.





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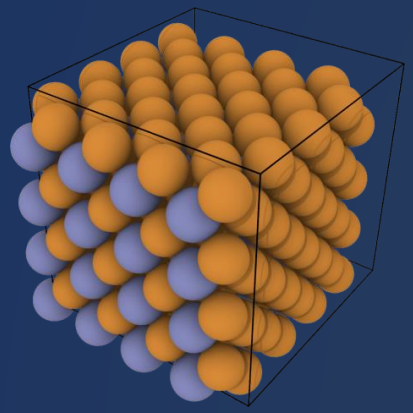
High-Dimensional Neural Network Potential for the Copper-Zinc System

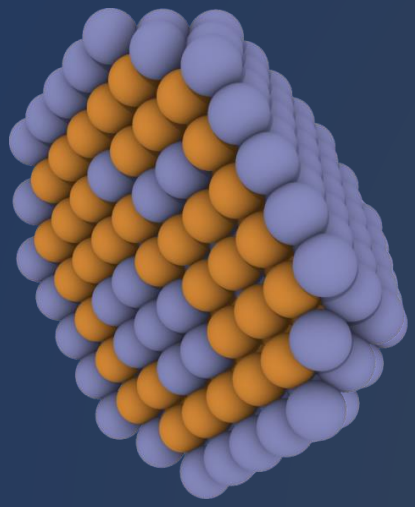
Jan Weinreich, Anton Römer, Martín Paleico, Jörg Behler
Theoretical Chemistry, Georg August Universität Göttingen

Session B
Poster number:
P081

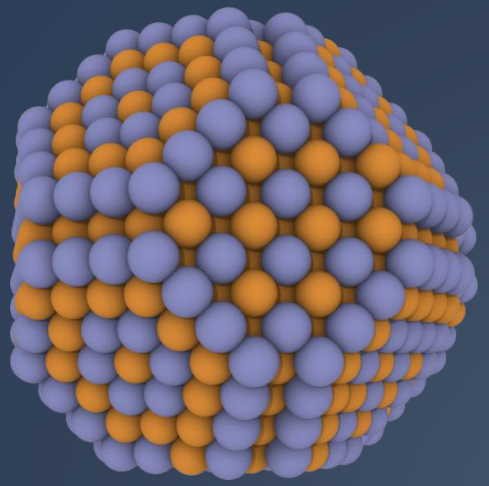
Large scale Metropolis Monte Carlo simulations for bulk brass and nanoparticles with the accuracy level of DFT



256 atoms bulk supercell



½ Cut of a 459 atom nanoparticle



1103 atoms ~ 2.8 nm

Poster Slam – Session A

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P113	Schwermann, C.; Doltsinis, N. L.	Computational Design of NHC-based Molecular Ratchets

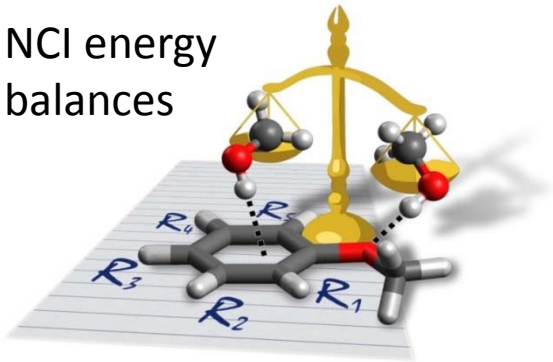
P089 – Benchmarking non-covalent interactions with *vibrational* spectroscopy

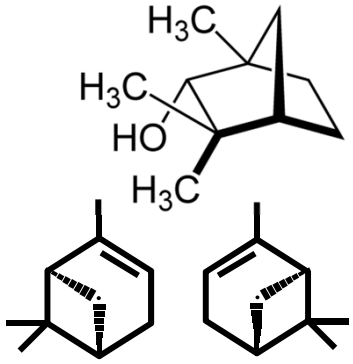
M. A. Suhm, H. C. Gottschalk, R. A. Mata, U. Göttingen

Angew. Chem. Int. Ed. **57** (2017) 11011
Benchmarking quantum chemical methods: are we heading in the right direction?

"...experimentalists should present posters at theoretical chemistry conferences..."

NCI energy balances





chirality recognition

BENCh RTG2455
bench.uni-goettingen.de

12 Ph.D. positions in theory and experiment – apply until Oct. 5 !

Poster Slam – Session A

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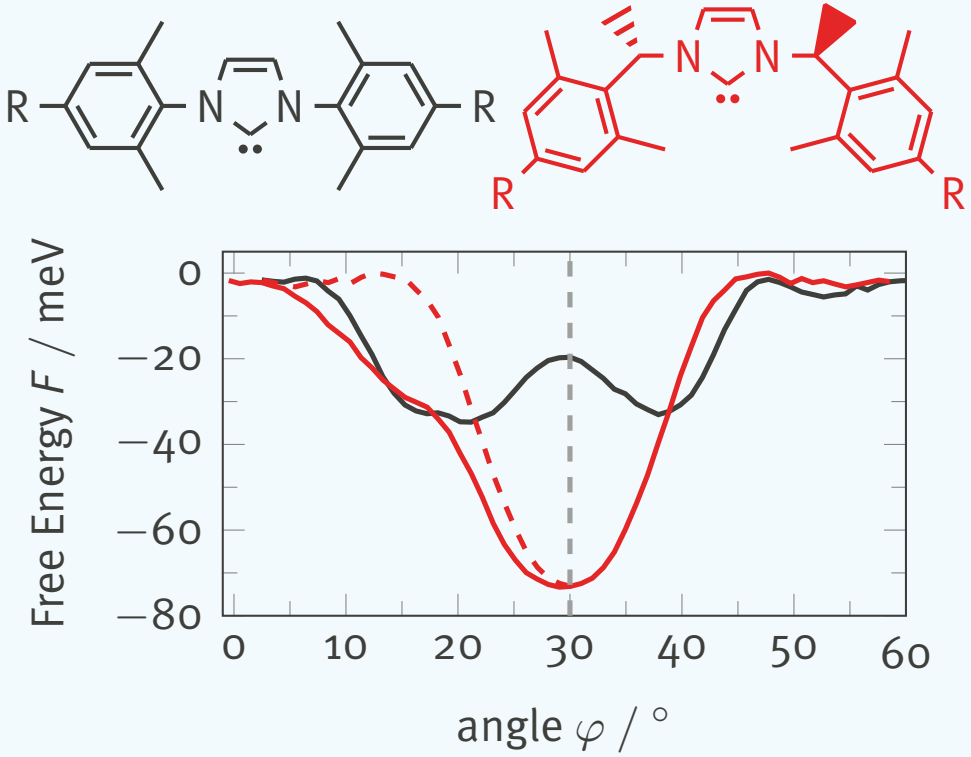
Computational Design of NHC-based Molecular Ratchets

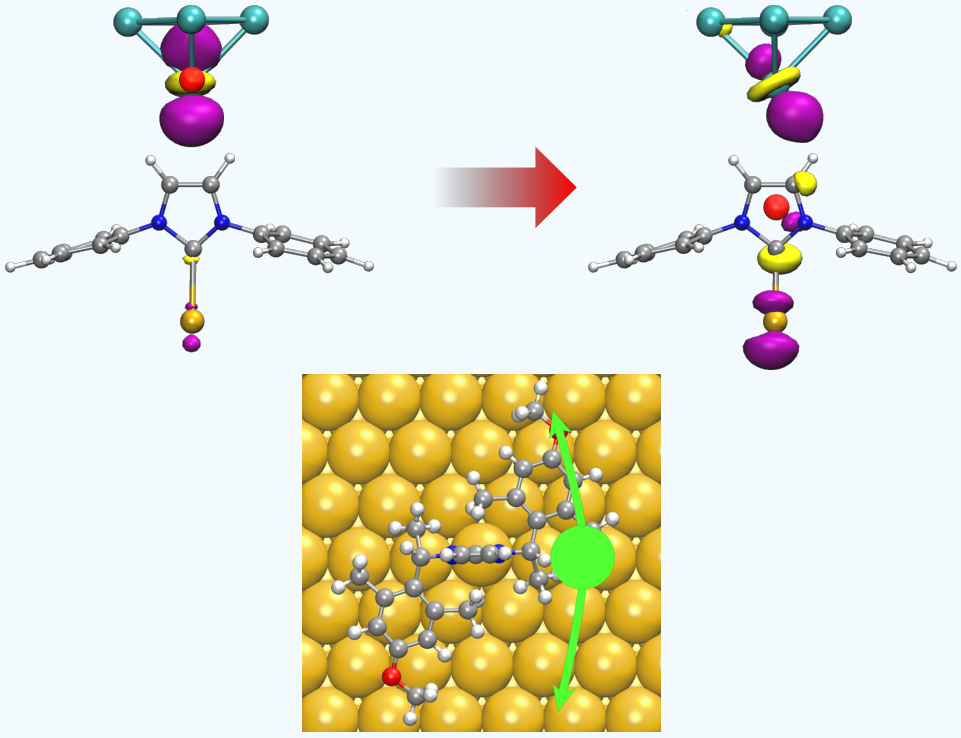
1. Design

- Rotational barrier is tuned with chiral ligands



2. Driving Force

- STM tip induces non-equilibrium dynamics



Christian Schwermann, Nikos L. Doltsinis

Poster Slam – Session A

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RUHR-UNIVERSITÄT BOCHUM

PBN: P125

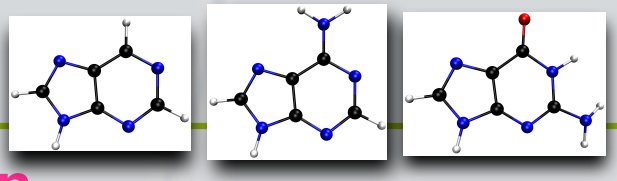
RUB

UV Absorption and Magnetic Circular Dichroism Spectra for Purinic Nucleobases in Aqueous Solution at COSMO-RI-CC2

Sarah K. Khani

Arbeitsgruppe Quantenchemie/Ruhr-Universität, Bochum 44780, Germany

Studying solvent effects on excited state properties



Method Development

An implementation of COSMO-RI-CC2 theory to calculate:

- ➡One- and two-photon absorption
- ➡MCD spectrum

Analysis of sum over state expression for Faraday $\mathscr{B}$ term

Application

Simulation of the UV-Vis & MCD spectra of purine, adenine and guanine in aqueous solution to investigate:

- ➡Relative positions of their electronic transitions
- ➡Capability of MCD in determining the relative stability of $\pi\pi^*$ transitions

Poster Slam – Session A

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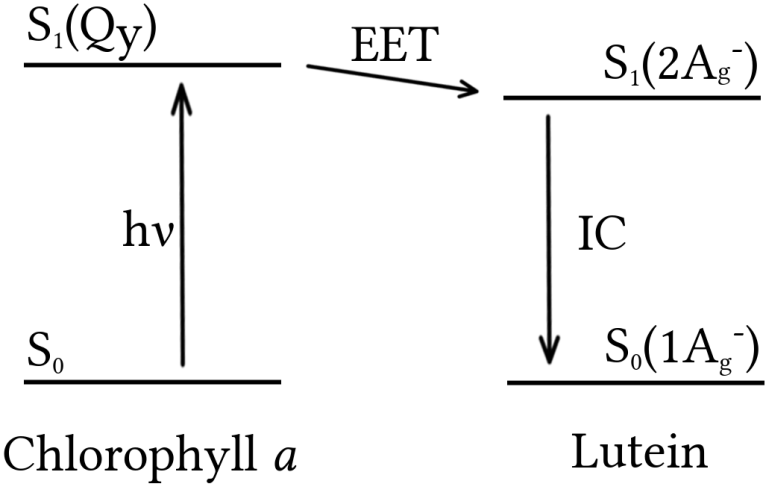
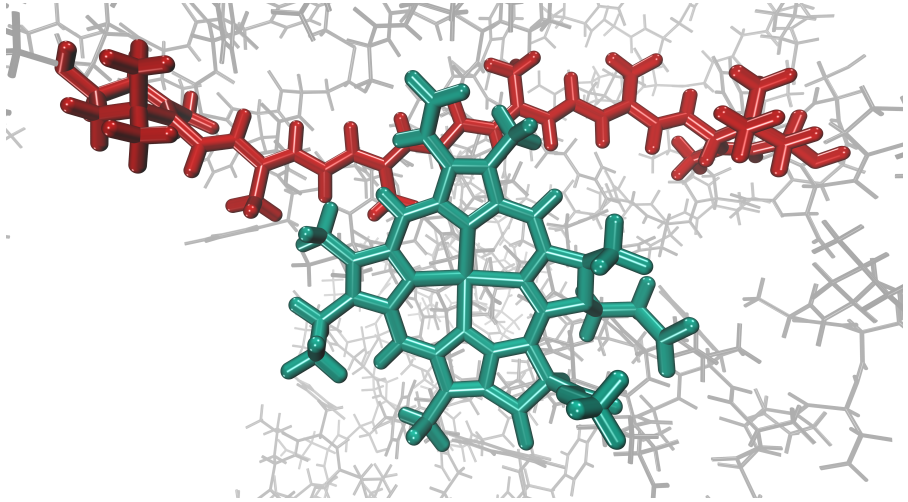
Exciton coupling in chlorophyll-lutein heterodimer of LHCII photoantenna is significantly affected by the size of MCSCF space for lutein calculation

P149





Various active spaces:

CAS[6,6]: |d|= 0.4 D

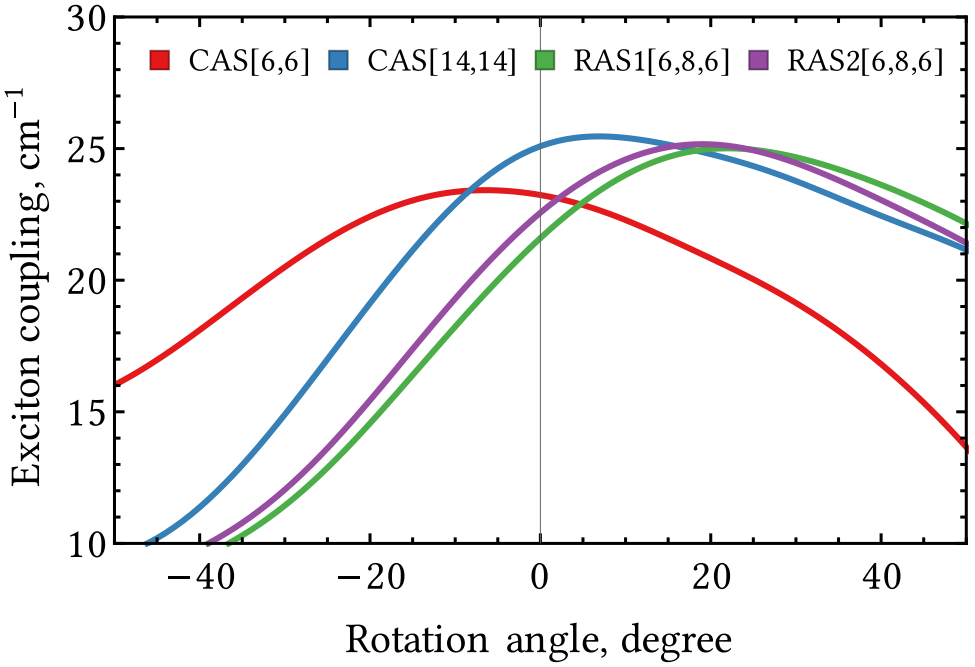
RAS2[6,8,6]: |d| = 0.06 D

Transition dipole moment varies by a factor of 6.7

CAS[6,6]: EET(0°)/EET(+20°) = 1.24

RAS2[6,8,6]: EET(0°)/EET(+20°) = 0.80

Completely different conclusions about the EET rate dependence on the pigments' mutual orientation



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