Poster Slam – Session B

P18	Manz, J.; Grohmann, T.; Haase, D.; Jia, D.; Yang, Y.	Quantum Effects on the Structures and Dynamics of Small Cyclic Molecular Rotors Imposed by the Molecular Symmetry Group
P20	Wedig, U.; Nuss, J.; Xie, W.; Yordanov, P.; Bruin, J.; Hübner, R.; Weidenkaff, A.; Takagi, H.	Hierarchical Bonding Pattern in the Thermoelectric Material $Ag_6Ge_{10}P_{12}$
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P150	Marefat Khah, A.; Reinholdt, P.; Kongsted, J.; Hättig, C.	The Impact of DNA-Confinement on The Photoisomerization of A Triazene: A PE-ADC(2) Study
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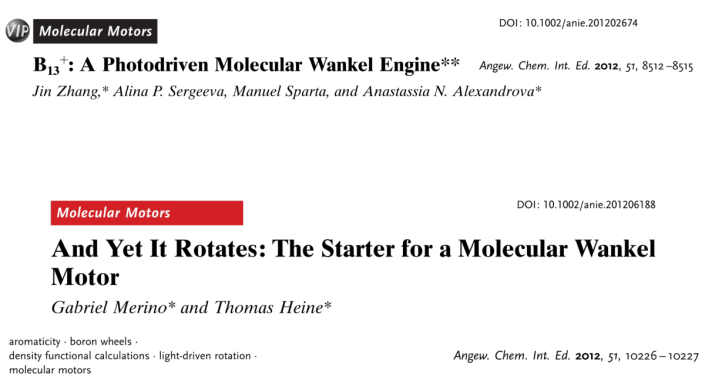
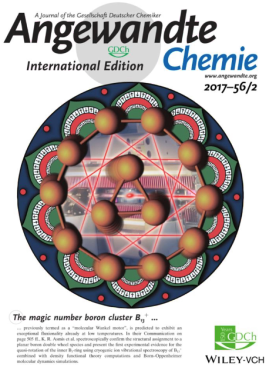
P018

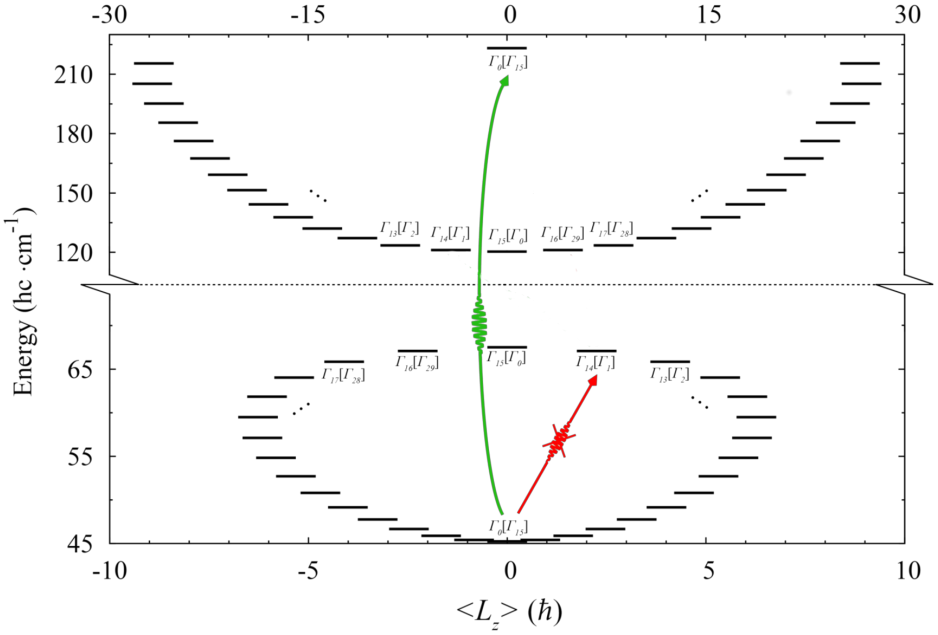
Quantum effects on the structures and dynamics of small cyclic molecular rotors imposed by the molecular symmetry group

Thomas Grohmann, Dietrich Haase, Dongming Jia, Jörn Manz, Yonggang Yang

Examples: H_2, CH_3, boron rotors ...







YES, they rotate, BUT laser ignition of the rotations is blocked by nuclear spins, and related MD simulations are inadequate.

Poster Slam – Session B

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A Fairy Tale: The Sleeping Beauty (Dornröschen)

Birth

$Ag_6Ge_{10}P_{12}$

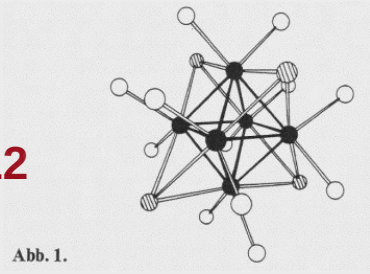

Abb. 1.

H. G. von Schnering, K.-G. Häusler; Rev. Chim. Mineral. ***13*** *(1976), 71.*

Childhood

Physical measurements in the mid 1980s
Optical, electrical, elastic and thermodynamic properties

Malediction of the evil fairy

'Three-dimensional band structure calculations on $Ag_6Ge_{10}P_{12}$ would be highly desirable in order to rationalize the electronic structure of the complex solid quantitatively for an explanation of the experimental results.'

'Unfortunately, so far, no precise bandstructure calculation has been performed….'

30 years sleeping

The Kiss of the Prince

See Poster 20

Poster Slam – Session B

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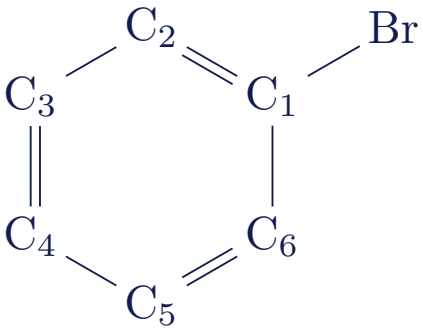
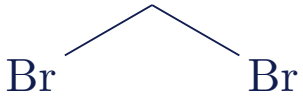
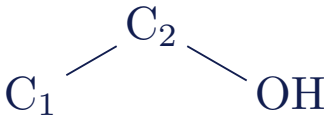
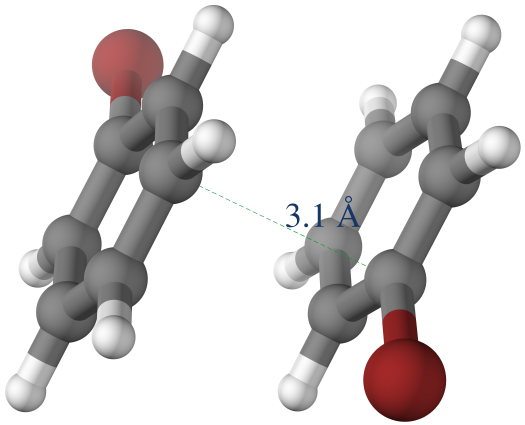
Isotope effects by the infinite improbability drive

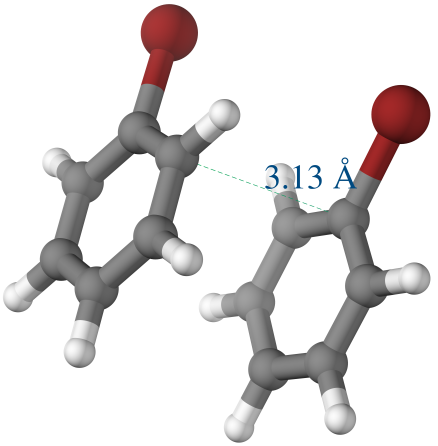
Poster 52











- Path integral molecular dynamics,
- Energy decomposition analysis,

Poster Slam – Session B

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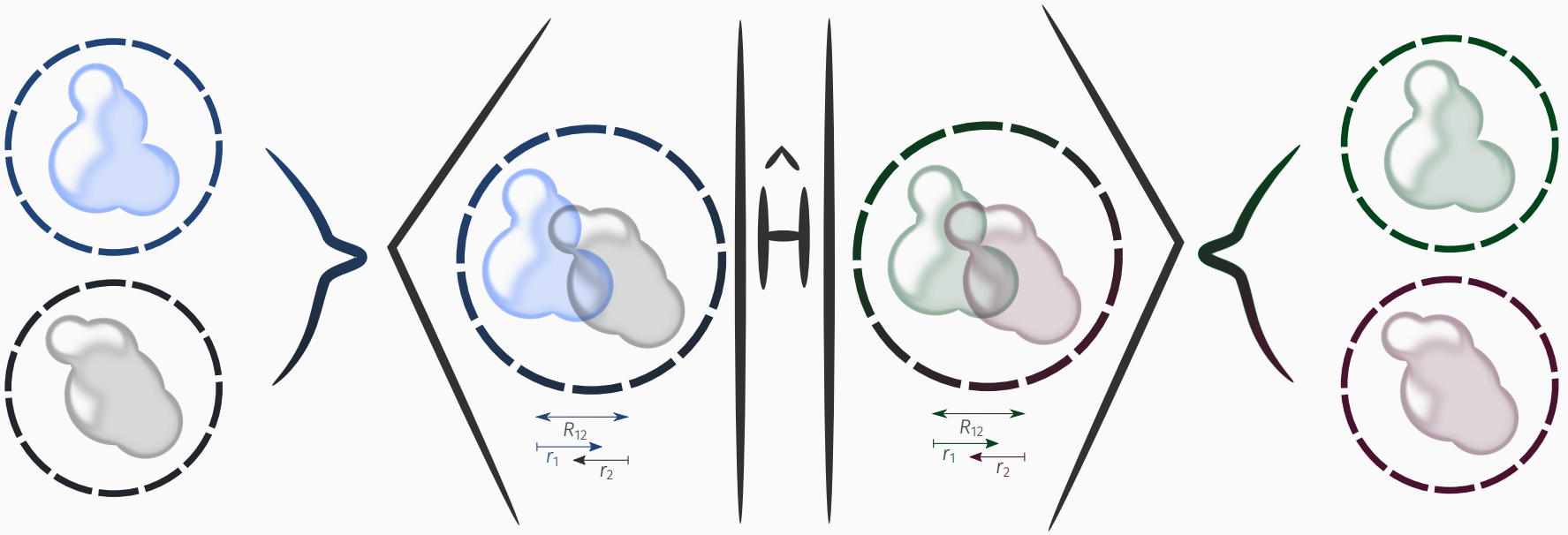
Electronic Coupling Integrals from Product Wave Functions: P062



$$\mathbf{H}_{2\times2} = \begin{pmatrix} H_{\mathrm{II}} & H_{\mathrm{IF}} \\ H_{\mathrm{IF}} & H_{\mathrm{FF}} \end{pmatrix}; \quad \mathbf{S}_{2\times2} = \begin{pmatrix} 1 & H_{\mathrm{IF}} \\ H_{\mathrm{IF}} & 1 \end{pmatrix} \Rightarrow V_{\mathrm{IF}} = \frac{\left| H_{\mathrm{IF}} - S_{\mathrm{IF}} \frac{H_{\mathrm{II}}+H_{\mathrm{FF}}}{2} \right|}{1-S_{\mathrm{IF}}^2}$$

Multi-state system: $\mathbf{V} = \mathbf{S}^{-\frac{1}{2}}\mathbf{H}\mathbf{S}^{-\frac{1}{2}}$

Poster Slam – Session B

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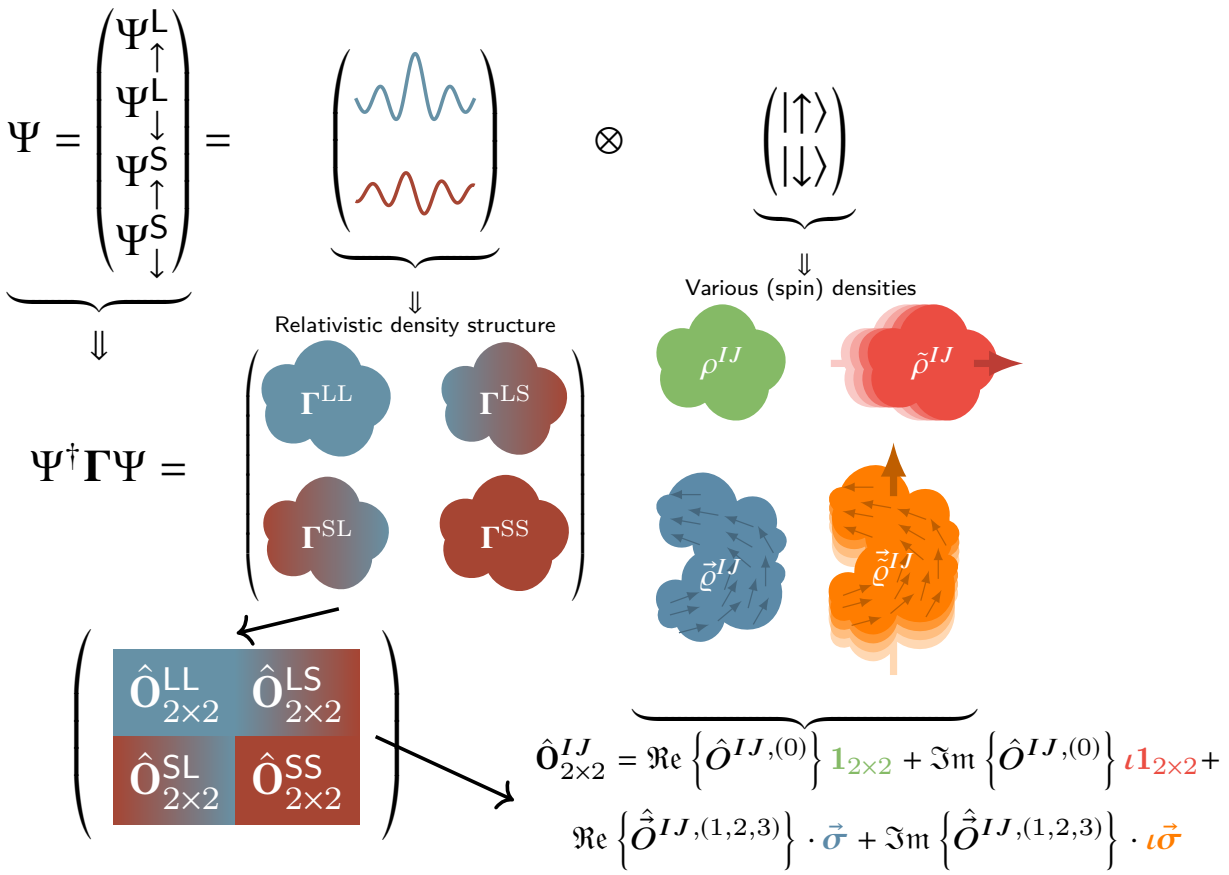
P066: Automated Property Calculation for Fundamental Physics Tests with Molecules

Custom one-electron properties from two-component wave functions



Poster Slam – Session B

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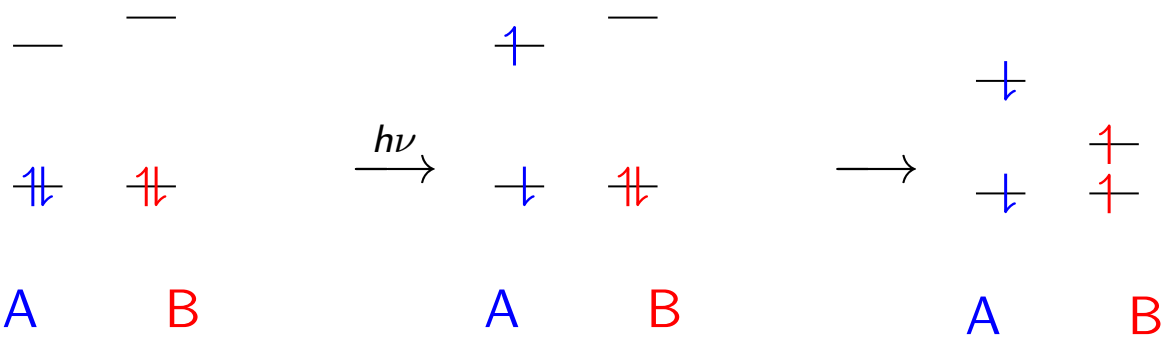
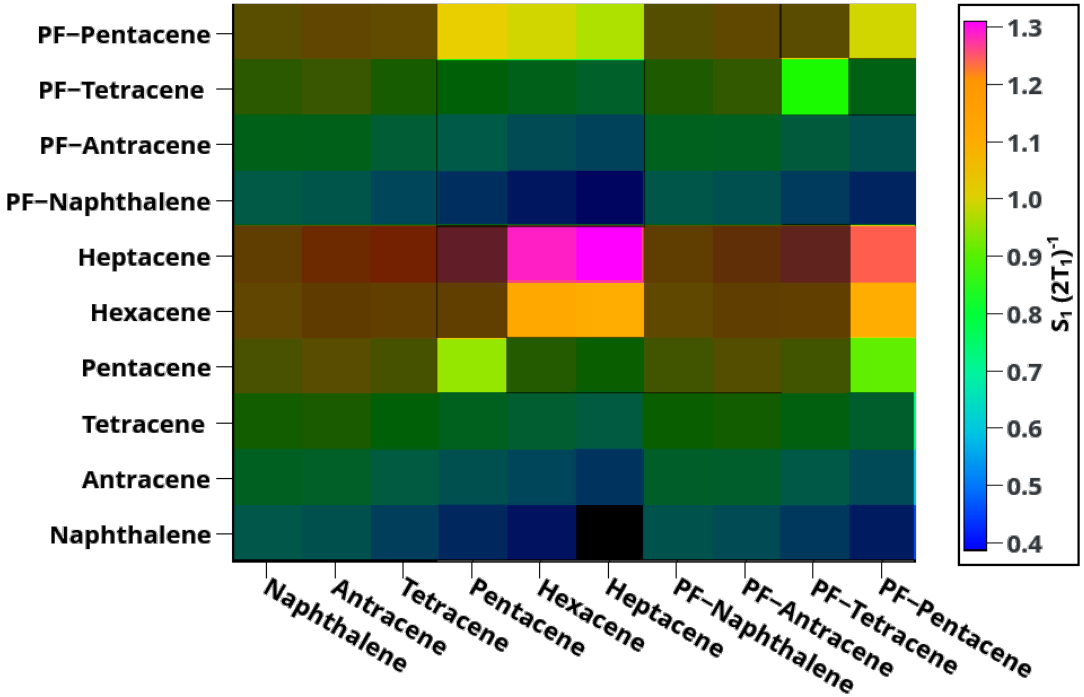
P070 - Molecular Energy Level Matching to Design Model Systems for Singlet Heterofission





Poster Slam – Session B

P70	Hansmann, A.-K.; Giesen, S. M.; Berger, R.	Molecular Energy Level Matching to Design Model Systems for Singlet Heterofission
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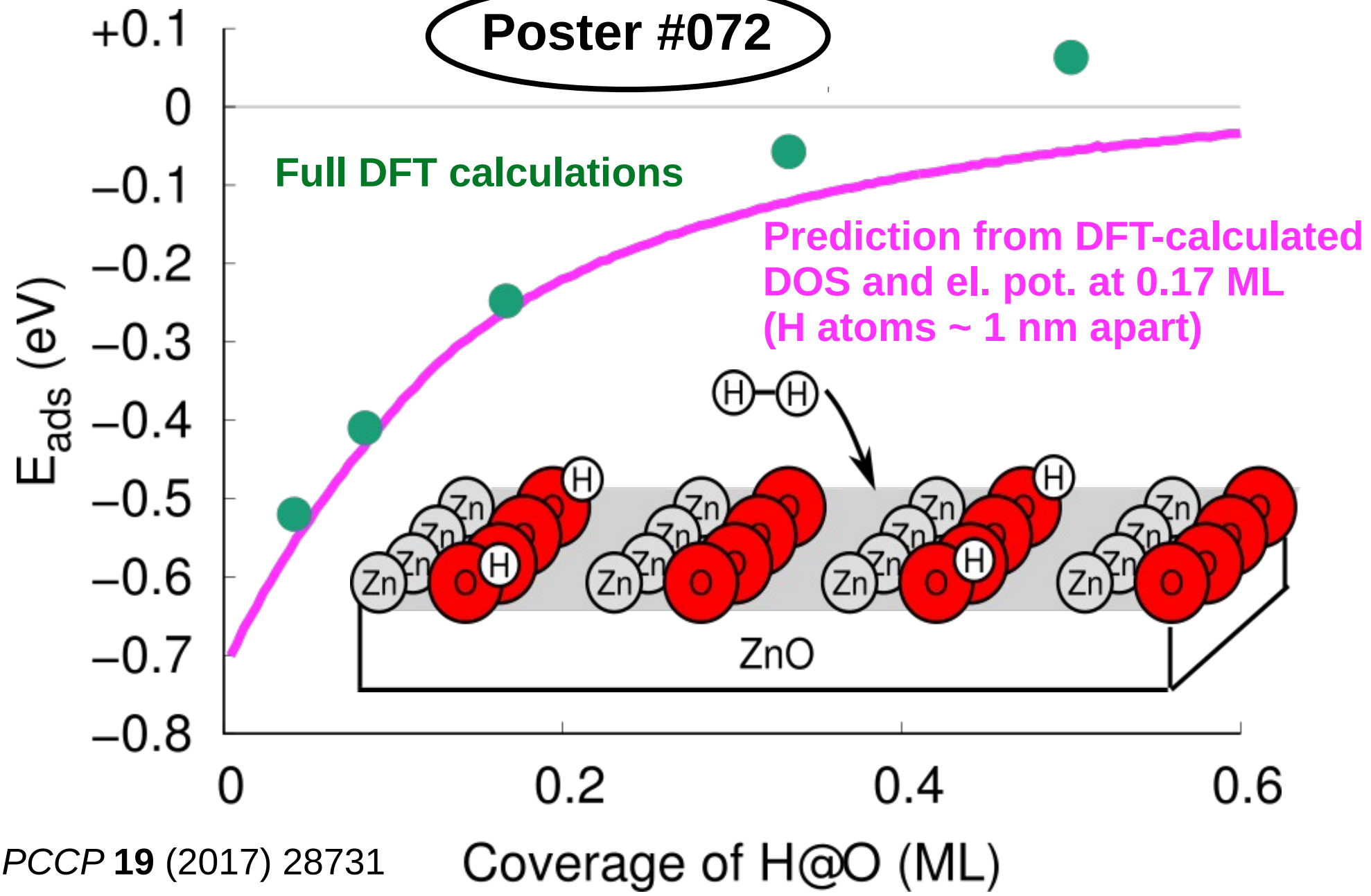
Surface phase diagram prediction from a minimal number of DFT calculations

Matti Hellström, Kersti Hermansson, Peter Broqvist, Jörg Behler

Poster #072



PCCP **19** (2017) 28731

Poster Slam – Session B

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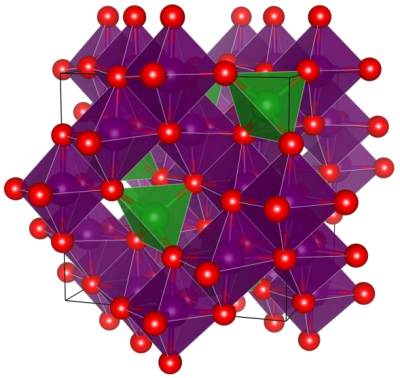
GÖTTINGEN

SFB 1073

A Neural Network Potential for Lithium Manganese Oxides

MARCO ECKHOFF, PETER E. BLÖCHL, JÖRG BEHLER

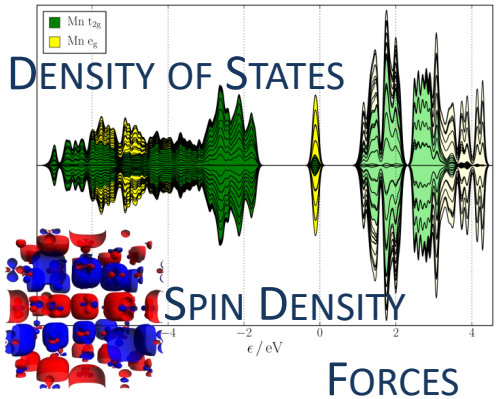
P082



$Li_xMn_2O_4$ spinel

DFT

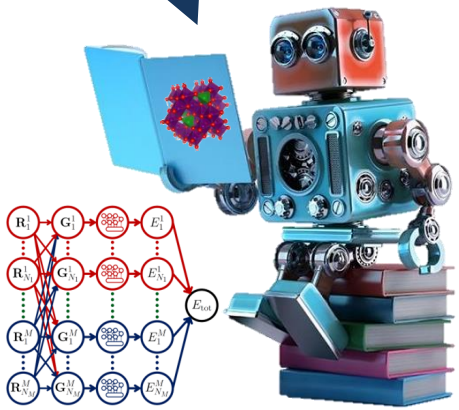
PBE0r



FORCES

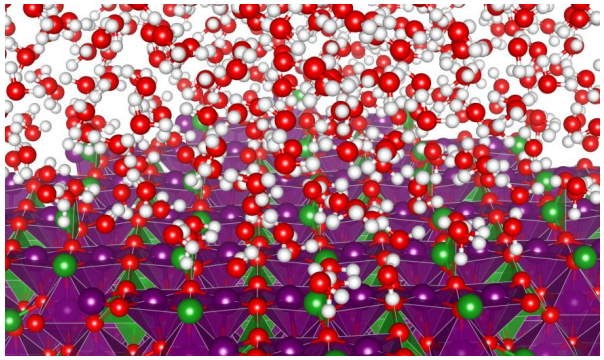
TOTAL ENERGY

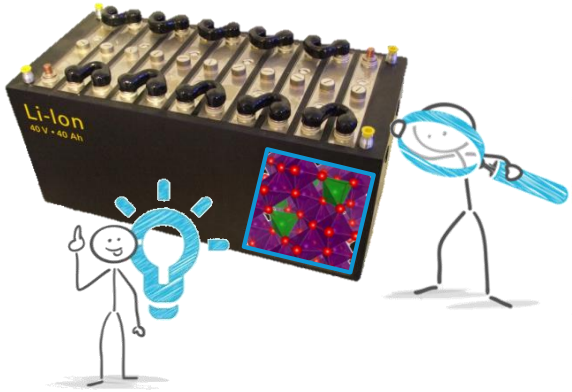
MACHINE-LEARNING



HIGH-DIMENSIONAL NEURAL NETWORK POTENTIALS

DFT





J. Behler, *Angew. Chem. Int. Ed.* **2017**, *56*, 12828–12840.
M. Sotoudeh, S. Rajpurohit, P. Blöchl, D. Mierwaldt, J. Norpoth, V. Roddatis, S. Mildner, B. Kressdorf, B. Ifland, C. Jooss, *Phys. Rev. B* **2017**, *95*, 235150.

Poster Slam – Session B

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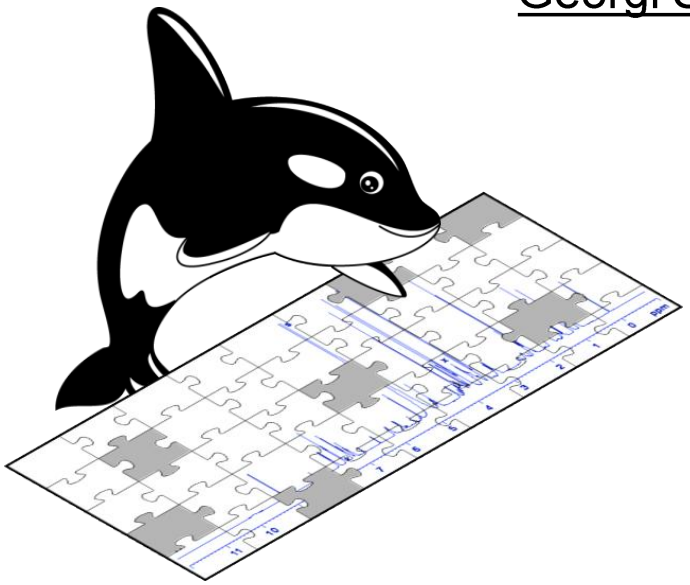
Efficient and Accurate Calculation of NMR Chemical Shifts

Georgi Stoychev, Alexander Auer, Frank Neese



$G_2 I_1 A_1 O_1 - D_2 F_4 T_1$

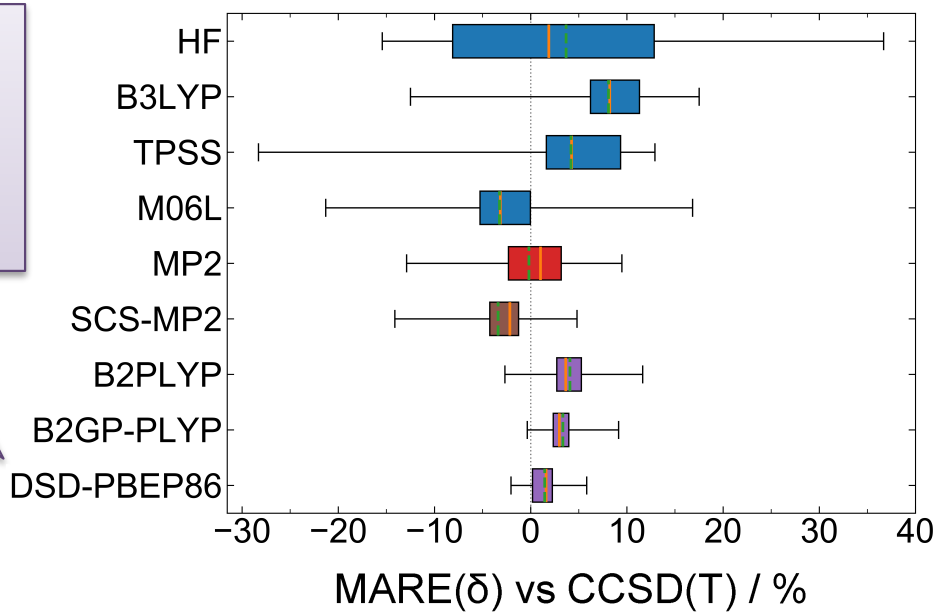
$G_2 I_1 A_1 O_1 - R_1 I_1 - M_3 P_3 2$

$G_2 I_1 A_1 O_1 - D_2 L_1 P_3 N_1 O_1 - M_3 P_3 2$

$G_2 I_1 A_1 O_1 - D_2 L_1 P_3 N_1 O_1 - C_3 C_3 S_1 D_2 (T_1)$

We are here

Double-hybrid DFT is better for NMR shifts than both MP2 and conventional DFT



AS SEEN ON P142

Poster Slam – Session B

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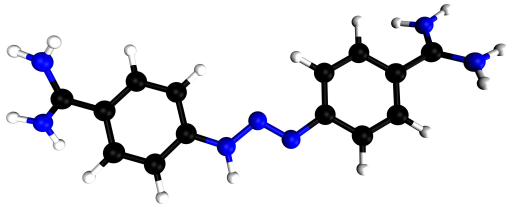
RESOLV
RUHR EXPLORES SOLVATION
CLUSTER OF EXCELLENCE - EXC 1069

RUB

The Impact of DNA-Confinement on The Photoisomerization of A Triazene: A PE-ADC(2) Study

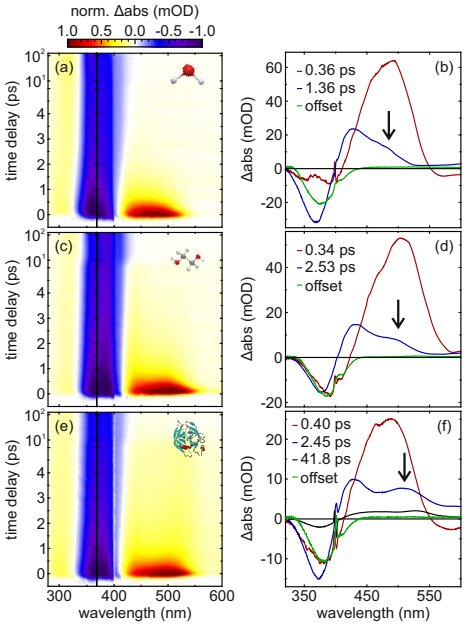
Alireza M. Khah, Theoretical Chemistry , Ruhr-Universität, Bochum

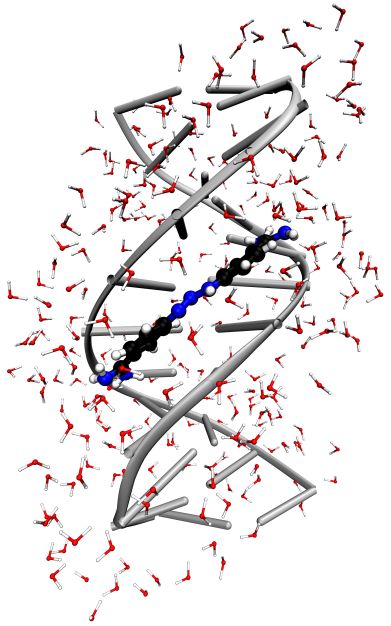


PBN: P150

Method Development

- First Implementation of PE-ADC(2) Excited State Energy And Analytical Gradients
- PE + (all-electron) ECPs Model To Avoid The Electron-Splitting Out Problem





Application

- Photoisomerization Pathways of berenil in solution
- The role of DNA to open new photochemical channels

Poster Slam – Session B

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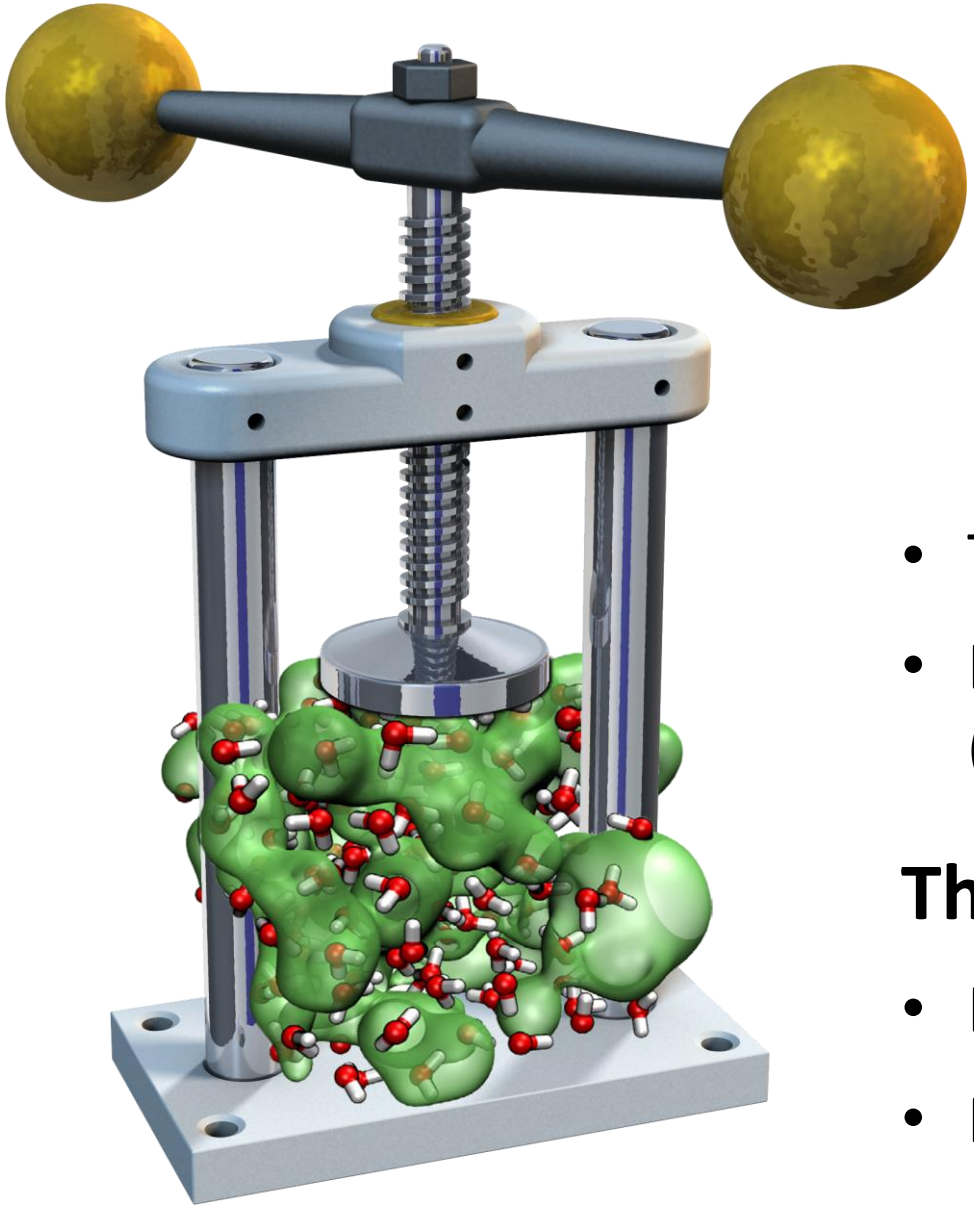
P158: Compressing Simulation Trajectories



M. Brehm, M. Thomas,
J. Chem. Inf. Model. **2018**, *accepted*.

- Trajectories are often large files
- Even worse for volumetric data (electron density CUBE files)

The BQB File Format:

- Lossless, random access
- Ratio of up to **40:1** *(vol. data)*
  up to **20:1** *(pos. data)*
- Free Software, GNU LGPL

Poster Slam – Session B

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