Intermolecular interactions and electron correlation

HEAD:

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GROUP MEMBERS:

PhD students: Michał Chojecki,
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RESEARCH PROFILE:

intermolecular interactions analysis, electron correlation in molecules, molecular properties

CURRENT RESEARCH ACTIVITIES:

- Modelling of intermolecular interactions of large molecules with state-of-art quantum-chemistry methods (symmetry-adapted perturbation theory, functional-group SAPT, interacting quantum atoms etc.)
- Method development of molecular properties of large molecules, including local electron correlation and molecular fragmentation approaches
- Investigation of electronic excited states of large molecules
- Development of Molpro suite of programs

SELECTED PUBLICATIONS:

1. G. Wälz, D. Usvyat, T. Korona, M. Schütz, A Hierarchy of Local Coupled Cluster Singles and Doubles Response Methods for Ionization Potentials, J. Chem. Phys. 144 (2016) 084117.
2. S. Yourdkhani, M. Chojecki, M. Hapka, T. Korona, Interaction of Boron-Nitrogen Doped Benzene Isomers with Water, J. Phys. Chem. A. 120 (2016) 6287-6302.
3. A. Heßelmann, T. Korona, Intermolecular Symmetry-Adapted Perturbation Theory Study of Large Organic Complexes, J. Chem. Phys. 141 (2014) 094107.
4. H. Dodziuk, T. Korona, E. Lomba, C. Bores, Carbon Nanotube Container: Complexes of $C_{50}H_{10}$ with Small Molecules, J. Chem. Theory Comp. 8 (2012) 4546-4555.
5. T. Korona, First-order exchange energy of intermolecular interactions from coupled cluster density matrices and their cumulants, J. Chem. Phys. 128 (2008) 224104.

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