Chałasiński Group

HEAD:

Prof. Grzegorz Chałasiński*, PhD DSc

GROUP MEMBERS:

Michał Hapka, PhD; Marcin Modrzejewski, PhD

RESEARCH PROFILE:

weak intermolecular interactions, density functional theory

CURRENT RESEARCH ACTIVITIES:

Our group is focused on the development and applications of electronic structure methods for weak intermolecular interactions. Recent works included advances in symmetry-adapted perturbation theory (SAPT) and density functional theory (DFT) methods based on Kohn-Sham formalism.

We introduced a variant of SAPT based on unrestricted Kohn-Sham treatment of the interacting monomers. Open-shell SAPT has been applied in a series of studies of small dimers relevant for ultracold chemistry. Moreover, we have investigated the possibility of merging the DFT-SAPT method with range-separated exchange-correlation density functional approximations. We have shown that the resulting LRC-SAPT method rivals the accuracy of the best-performing DFT-SAPT approaches.

Our work on improving hybrid semilocal DFT approximations has been focused on removing unnecessary empirical parameters and merging DFT with a proper description of long-range correlation effects. We devised a method for converting an arbitrary GGA or a meta-GGA functional into a range-separated hybrid which is free from DFT's shortcomings for, e.g., charge transfer systems. We have also analyzed the performance of different DFT approaches for calculations of many-body interaction energies. Our work established which nonadditive interaction energy components pose a considerable challenge even for best-performing modern DFT functionals. Works to properly account for these effects in the existing DFT approximations are under development in our group. Our current research involves merging DFT with the random-phase approximation model for electron correlation.

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SELECTED PUBLICATIONS:

1. M. Hapka, Ł. Rajchel, M. Modrzejewski, R. Schäffer, G. Chałasiński, M.M. Szczęśniak, The nature of three-body interactions in DFT: exchange and polarization effects, J. Chem. Phys. 147 (2017) 084106.
2. M. Modrzejewski, M. Hapka, G. Chałasiński, M.M. Szczęśniak, Employing range separation on the meta-GGA rung: New functional suitable for both covalent and noncovalent interactions, J. Chem. Theory Comput. 12(8) (2016) 3662-3673.
3. M. Hapka, Ł. Rajchel, M. Modrzejewski, G. Chałasiński, M.M. Szczęśniak, Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory, J. Chem. Phys. 141 (2014) 134120.
4. M. Modrzejewski, G. Chałasiński, M.M. Szczęśniak, Range-separated meta-GGA functional designed for noncovalent interactions, J. Chem.Theory Comput. 10(10) (2014) 4297-4306.
5. J.V. Koppen, M. Hapka, M. Modrzejewski, M.M. Szczęśniak, G. Chałasiński, DFT for gold-ligand interactions: Separating true effects from artifacts, J. Chem. Phys. 140 (2014) 244313.
6. M. Hapka, G. Chałasiński, J. Kłos, P. S. Żuchowski, First-principle interaction potentials for metastable He(^{3}S) and Ne(^{3}P) with closed-shell molecules: Application to Penning-ionizing systems, J. Chem. Phys. 139 (2013) 014307.
7. M. Modrzejewski, Ł. Rajchel, G. Chałasiński, M.M. Szczęśniak, Density-dependent onset of the long-range exchange: A key to donor–acceptor properties, J. Phys. Chem. A. 117(45) (2013) 11580-11586.