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Noncovalent interactions in bio- and nanosciences: quantum mechanical aproach

Noncovalent interactions play an important role in chemistry, physics and biology. Reliable characteristics like stabilization energy, structure and vibrational frequencies are obtained using composite coupled cluster schemes which offer the possibility of improving the accuracy of results obtained by adding excitation operators of increasing order. It was shown that already CCSD(T)/CBS method yields an accurate and reliable description of noncovalent interactions, yet is only applicable to systems with several tens of atoms. Lower-level methods like DFT or semiempieical QM (SQM) should be parametriezed or verified and here the databases of accurate stabilization energies and geometries developed in our laboratory (S22, S66, X40 and L7) play an indispensable role. Binding free energy for host-guest and protein-ligand complexes is constructed as a sum of gas-phase interaction energy (ΔEint), change of desolvation free-energy (ΔΔGsolv), change of the conformational free energy of both components (ΔGconfw) and entropy term (eq. 1): $\Delta G_w \approx \Delta E_{int} + \Delta\Delta G_{solv} + \Delta G_{confw} - T\Delta S$ (1). Because of the size of systems investigated the DFT-D, and PM6 or SCC-DF-TB SQM methods combined with COSMO technique were considered. Performance of these methods was verified by comparison of interaction energies of model complexes with the benchmark values obtained from CCSD(T) and MP2.5 methods. Applicability of procedures described is demonstrated for evaluation of binding free energies of several extended systems like host – guest, protein – ligand and surface – admolecule ones.

Recent Publications

1. Rezac J and Hobza P (2016) Benchmark calculations of interaction energies in noncovalent complexes and their applications. Chem. Rev. 116(19):5038-5071.
2. Hostas J et al. (2016) A nexus between theory and experiment: non-empirical quantum mechanical computational methodology applied to cucurbit[n]uril.guest binding interactions. Chem. Eur. J. 22(48):17226-17238.
3. Sigwalt D et al. (2017) Unraveling the structure-affinity relationship between Cucurbit [n]urils (n=7, 8) and cationic diamondoids. J. Am. Chem. Soc.139():3249-3258.
4. Pecina A et al. (2017) QM/COSMO Scoring function at the DFTB3-D3H4 level: unique identification of native protein-ligand poses J. Chem. Inf. Model. 57:127-132.

Biography

Pavel Hobza (dr.hc, FRSC) obtained his PhD (1974) from the Institute of Physical Chemistry of the Academy of Science of the Czech Republic. He is a Distinguished Chair at the Institute of Organic Chemistry and Biochemistry of the Academy of Sciences of the Czech Republic, Prague, Czech Republic. His research team works on noncovalent interactions and their applications in bio- and material sciences, databases of accurate interaction energies and on *in silico* drug design. He has co-authored 4 books, more than 450 papers and 35 review papers in peer-reviewed journals, his H-index (WOS) is 98, sum of Times Cited is more than 35,000. He was awarded by "Highly Cited Researcher" in chemistry during 2014-2016 (Thomson Reuters, later Clarivate Analytics) and Schrödinger Medal in 2017 (World Association of Theoretical and Computational Chemists).

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