Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Internal Seminar

Rapid and accurate composite ab initio models for high-throughput computation of molecular thermochemistry across chemical space

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The MolDis computational chemistry Big Data analytics platform (https://moldis.tifrh.res.in/) aims at developing various domain specific molecular and materials datasets. For molecular datasets relevant to organic- and bio-chemical applications, desirable properties include thermochemical and kinetic stabilities. Reliable estimations of these properties require a degree of accuracy comparable to experimental uncertainties. The talk will comment on state-of-the-art composite quantum chemistry methods that yield highly accurate thermochemical properties by exploiting additivity of electronic energies.

Of key importance to this project is to identify among the existing computational models one that offers accurate heat-of-formation, ionization energy, electron affinity, proton affinity, non-bonding interaction energy and pKa. The study focuses on the critical evaluation of the additivity assumption in the composite procedure G4(MP2) and proposes modifications to this scheme to reduce the computational cost further without compromising accuracy and transferability across various chemical datasets. The proposed strategy is based on the theories of resolution-of-identity expansion of two-electron Coulomb integrals and local coupled-cluster method which offers the best speed-to-accuracy trade-off. Preliminary results indicate that this new method forecasts molecular energetics with in about 1 kcal/mol accuracy compared to pruned experimental datasets and enables high-throughput computation of molecular thermochemistry.

Tuesday, Jun 4th 2019

2:30 PM (Tea/Coffee at 2:00 PM)

Seminar Hall, TIFR-H