Contribution ID: **113** Type: **Talk**

Electron density in uncovering reaction mechanism

Tuesday, 1 December 2020 11:00 (30 minutes)

A REP-FAMSEC (reaction energy profile–fragment attributed molecular system energy change) protocol designed to explain each consecutive energy change along the reaction pathway will be briefly described. Electron density-dependant energy components defined in the Interacting Quantum Atoms (IQA) energy partitioning scheme are used to explore interactions between meaningful polyatomic fragments of a molecular system. By quantifying energetic contributions, as defined within the REP-FAMSEC method, one can pin-point fragments (atoms) leading to or opposing a chemical change. Usefulness of the REP-FAMSEC method will be demonstrated, as a case study, on the proline catalysed aldol reaction for which a number of mechanisms is being debated for over four decades. Relative stability of S-proline conformers, their catalytic (in)activity and superior affinity of the higher energy conformer to acetone will be fully explained on an atomic and molecular fragment levels. Importance of the CHPC in running high level, time-, and resource-demanding quantum computing will also be advocated.

Student?

No

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Session Classification: HPC Applications

Track Classification: Computational Chemistry