Chemical Bonding from Wavefunction Analysis with APOST-3D

Martí Gimferrer[1]

[1]Institut für Physikalische Chemie, Georg-August Universität Göttingen, Tammannstraße 6, 37077 Göttingen, Germany

E-Mail presenting author: marti.gimferrerandres@uni-goettingen.de

The open-source APOST-3D software[1] features a large number of wavefunction analysis tools to connect classical chemical concepts with the electronic structure of molecules. APOST-3D relies on identifying the atom in the molecule (AIM), and most chemical bonding tools are implemented in a way that they can be used in combination with any chosen AIM (Hilbert- or real-space).

Besides conventional population analysis of the density and bond orders, APOST-3D implements different schemes for oxidation state (OS) assignment (EOS, OSLO), molecular energy decomposition schemes, and local spin analysis. The APOST-3D platform offers a user-friendly interface and a comprehensive suite of state-of-the-art tools to bridge the gap between theory and experiment. It provides resources for both seasoned computational chemists and researchers with a focus on experimental work.

Herein, we will provide an overview of the code capabilities with illustrative examples, emphasizing the OSs elucidation with EOS[2] and OSLO[3] and rationalization of Lewis acid/base reactivity in main group compounds from these calculations.[4]

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