Abstract Submitted
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Visualizing Valence Electron Structure[1] AERYK KUNA, ANTONIO CANCIO, Ball State University — The purpose of this research is to effectively model and understand Density Functional Theory (DFT). DFT uses the electron density to model the ground state electronic structure of atoms, molecules, and solids. We calculate and visualize the gradient of the electron density, its Laplacian, and the kinetic energy density, also derived from the electron density, for the AE6 test set of molecules. This set of six molecules accurately represents the DFT prediction of atomization energies of a plethora of molecules. Calculations were done using the ABINIT DFT code. Pseudopotentials were used to represent the individual atom cores, keeping an accurate representation of valence interactions. By using these density- derived functions we can better visualize and interpret intermolecular phenomenon caused by electron interactions, like the effects of a triple bond on the entire structure of the molecule, or the effect of electron affinity of an individual atom within a molecule. These physical variables are used in DFT to help predict the electron-electron interaction energy of a molecule, and knowing how they relate to each other may help better model this. Ultimately, we hope to effectively use our results to understand and improve the Density Functional method for modeling electronic structure.

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