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Visual Analysis of DFT Functionals K.M. FLURCHICK, PATRICK MCCARTER, North Carolina A&T State University — In this work, various functionals for Density Functional Theory calculations are investigated. The computed electron density, molecular geometry and other properties are compared to experimental and CCSD(T) calculations to determine the effectiveness of each functional. In this work, the electron density differences between each functional, the CCSD(T) results and experimental values are analyzed both visually and numerically. Small carbon based molecules are used to study the different functionals including single, double and triple bonds. The properties considered in this work include the geometry, energies, ionization potential and gradients of the electron density.

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