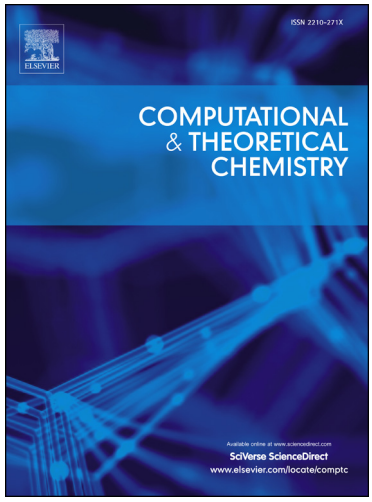

Simple Empirical Models for Predicting Electron Correlation in Small Molecular Systems

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Simple Empirical Models for Predicting Electron Correlation in Small Molecular Systems

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Abstract

Simple empirical models that can account for the electron correlation energy in molecular systems have been investigated. The aim of these models is to describe the electron correlation energy as a function of properties, such as the Coulomb and kinetic energies, obtained using the computationally efficient Hartree-Fock method with the 6-31G(d,p) basis set. Correlation energies for a set of 56 small molecules were also modelled as linear functions of the total number of electrons and the number of opposite-spin electron pairs for comparison. We found that the best model is one based on the density at the nucleus with an accuracy comparable to the LYP correlation functional. Considering the simplicity of the models investigated, their computational efficiency could be advantageous over more rigorous, yet computationally expensive correlated methods.

Keywords: , Electron Correlation, Hartree-Fock, Correlation Energy Modeling, Coulomb Correlation