

Abstract Submitted
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Quantum Entanglement and Electron Correlation in Molecular Systems¹ HEFENG WANG, SABRE KAIS, Department of Chemistry, Purdue University, West Lafayette, IN, 47906 — We study the relation between quantum entanglement and electron correlation in quantum chemistry calculations. We prove that the Hartree-Fock (HF) wave function does not violate Bell's inequality, thus is not entangled while the configuration interaction (CI) wave function is entangled since it violates Bell's inequality. Entanglement is related to electron correlation and might be used as an alternative measure of the electron correlation in quantum chemistry calculations. As an example we show the calculations of entanglement for the H₂ molecule and how it correlates with the traditional electron correlation, which is the difference between the exact and the HF energies.

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Hefeng Wang

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