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Electronegativity in quantum chemistry

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Abstract

The possibility is discussed for determination of chemical potential (electronegativity) of an electron-nucleus system in terms of the quantum-mechanical density functional theory (DFT). The principle of complete leveling of chemical potentials of natural orbitals, formulated in the framework of DFT, cannot be regarded now as justified. The calculation of electronic chemical potential via difference schemes still remains the only procedure suitable for estimation of this quantity by quantum-chemical methods.

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