## half-electron (HE) model

An approach to treating open-shell molecular systems by a closed-shell formalism which utilizes the similarity between the SCF equations (see Hartee-Fock method) and those for a fictitious closed-shell system in which the odd electron is replaced by two half-electrons. The model is applied for calculating energies of radicals by use of semi-empirical quantum mechanical methods.

1999, 71, 1941

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