

Effect of Long-range Electronic Correlation on the Organic pi Electron Molecular Systems and Long-range Electronic Correlation Energy for Excited States (ISCOM 2009)

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A general formula for long-range electronic correlation energy with off-diagonal interactions for pi electron systems has been given, which is beyond the nearest-neighbor electron-electron interactions[1]. Now a formula for long-range electronic correlation energy for excited states for pi electronic systems is given at the first time, by which we can discuss the effects of the long-range electronic correlations on problems of exciton and polaron in pi electron systems. We discussed the effects of the long-range electronic correlation on band gap, charge transfer along the molecular chain, and polarization.

The off-diagonal electron-electron interactions are clearly related to the long-range correlation effects. It is found that the effects of the off-diagonal interactions W and X on the correlation energies are opposite, but the influence of X on the correlation energies is counteracted by the integral J due to $|X| \sim |J|$, and the correlation energies decrease with increasing the screening effect. According to the general formula of the long-range correlation energy, we have put forward to a correlation Hamiltonian. Due to the possible connection of the off-diagonal interaction $X (< 0)$ to superconductivity and the connection of the off-diagonal interaction W to ferromagnetism, these correlation effects maybe imply an significance to the pi electron systems with such physical properties.

Presentation preference

Poster

Category:

2 Theory, Modeling and Computation

[1] H. Zhao, Eur.Phys.J. B54, (2006) 11