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DMRG Studies on Properties of Undoped and Doped Molecule-Based Ferromagnetic Chain

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Abstract: By using density matrix renormalization group (DMRG) method a model for organic molecule-based ferromagnetic chain is proposed. It is found that the ground states of undoped and doped systems both exhibit ferrimagnetic ordering. The e-e repulsion plays an important role in the stability of the ferromagnetic state either in doped system or undoped system. For the undoped system, each unit cell contains half of the total spins, which is consistent with Lieb's theorem. It is convinced that when the system is doped with one electron, a charge density wave is excited, which decreases the amplitude of spin density wave, therefore acting against the stability of ferromagnetic state.

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Key words: DMRG, antiferromagnetic exchange, SDW, spin density, undoped, doped

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