

Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

Mardi 21 Juin à 14:30

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DMRG Studies of the Ground and Low-Lying Excited States in Fused Carbon Ring Systems

Organic molecules with extended p-conjugation are important as active materials in molecular electronic devices. Modeling the low-lying electronic states in these systems is important for tailoring molecules for applications. The p-electrons in these materials experience strong long-range correlations as the systems are semiconducting and quasi one-dimensional. The electron states in these molecules are modeled using the Pariser-Parr-Pople (PPP) model which is a long-range Hubbard model introduced in chemistry in the early fifties. We show that the PPP model of quasi-one-dimensional system can be studied by using the DMRG method as the long-range interactions are site diagonal and do not increase the entanglement of the states even though the interactions in the model are topologically higher dimensional. We discuss one particular class of conjugated systems which are fused ring systems. Graphene nano ribbons (GNRs) belong to this class of systems. We show that in some systems, the ground state spin depends upon the number of fused units in the system as well as on the topology of the system. We discuss an efficient symmetrization method for targeting experimentally accessible excited electronic states. We discuss the properties of these states to demonstrate the effect of electron correlations.

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