Mapping of the DFT spin configuration energies of chromium-based molecular rings onto the energy structure of Falicov-Kimball model

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A comprehensive study of electronic and magnetic properties of a recently synthesized family of octo- and nonametalic chromium-based homo- and heteronuclear molecules is presented, using DFT and Falicov-Kimball (FK) model approach.

The magnetic moments are calculated and the spin charge density maps for various spin configurations are discussed. The exchange coupling parameters between transitional metals ions are extracted. In addition, the HOMO and LUMO orbitals are plotted and discussed. It is demonstrated that the energies of the spin configurations can be reproduced by the FK model with a given set of parameters. For all molecular rings considered, the ground state corresponds to the antiferromagnetic configuration and the ferromagnetic configuration yields the highest energy.