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Magnetism driven by resonating valence bonds in low dimensional conjugated systems SEFA DAG, VINCENT MEUNIER, WILLIAM A. SHELTON, Oak Ridge National Laboratory — We report the theoretical study of the electronic and magnetic properties of two dimensional metal-π tconjugated complex (XPc) constituted of a transition metal ion and a benzene bridge as $\pi-$tconjugation. Our investigations have been carried out by means of electronic structure calculations based on density functional theory within the local density approximation and led to find the many important ground state properties. In particular they result in an accurate description of the two-dimensional electronic structure, the insulating behavior, and the magnetic order in this system. Furthermore we reach the conclusion that band theory is well suited to describe the magnetic structure investigated here, since it possesses localized moments. We discuss the implications of our results on the magnetism of XPc structures from the view point of charge and spin density distributions, shape of the state orbitals, and their occupation numbers.

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