

Abstract Submitted
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Hückle π -electron theory of self-assembled metalloporphyrin films

W. SCHWALM, J. MORENO, University of North Dakota, A. BRANDT, Moorhead State Univ. — Porphyrin-based thin films including transition metal ions can be formed by self-assembly (Y. Ni and Q. Huo, *J. of Porphyrins and Phthalocyanines* **9**, 275 (2005)). They have significant magnetic and optical properties. Assuming that the structures are planar and two-dimensionally periodic, the π -electron theory, though highly approximate, may give some rough insight into their electronic properties. We model the two-dimensional array of metalloporphyrin molecules using a double-exchange Hamiltonian, that couples the local moments on the metal ions with the metal-like extended π -orbitals. Within a parametrized Local Combination of Atomic Orbitals (LCAO) approximation the electronic wave-function is treated in a minimal basis of states odd in reflection through the plane of the molecule. Local Density of States and other simple properties are computed by Green function methods. The support surface interaction breaks the reflection symmetry and contributes self energy. This effect is included through a simple model approximation.

Juana Moreno
University of North Dakota

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