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Application of atomic-orbital projections to the study of the electronic properties of metal-organic frameworks LUIS AGAPITO, Department of Physics, University of North Texas, ARRIGO CALZOLARI, ANDREA FERRETTI, Istituto Nanoscienze CNR-NANO-S3, Modena, Italy, MARCO NARDELLI, Department of Physics, University of North Texas — Metal-organic frameworks (MOF) are a new class of artificial crystalline materials. Because of their flexibility for synthesis and instrinsic ultrahigh surface area and porosity, MOFs show superior performance in gas storage, catalysis, and sensing applications. We use an efficient projection of plane-wave wavefunctions onto atomic orbitals for studying the electronic properties of these intriguing materials. The present scheme harnesses the robust periodic algorithms and systematic convergence of the plane-wave method for an atomistic electronic (Landauer conductance) and chemical (charge transfer, bond and atomic charge) analysis that provides guidelines for the design of MOF electronic materials.

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