 ICCES, vol.17, no.4, pp.123-123

The localization / delocalization dilemma in the electronic structure of d- and f- element oxides

Richard L. Martin

Summary

The electronic structure of many of the oxides containing d- and f-elements has long been a challenge for theory. For example, the traditional workhorses of density functional theory, the local density approximation (LDA) and the generalized gradient approximations (GGA), predict most of these systems to be metallic, when in fact they are insulators with band gaps of several eV. These problems reflect the localization/delocalization dilemma faced in systems with weak overlap and seem to be largely overcome by the new generation of hybrid density functionals developed for molecular studies. Only recently has it been possible to apply these functionals to solids but in the cases studied thus far we find a distinct improvement. The hybrid functionals predict the correct insulating ground state, band gap, lattice constant and magnetic behavior at 0K, where known. I will review the origin of the problem, how hybrid functionals differ from traditional ones, and recent applications to MnO, CeO2, Ce2O3, and the actinide oxide series AnO2, An = Th ... Es.