Optimised projections for the Ab initio simulation of large and strongly correlated systems

O'Regan, David D., author

Abstrak

The dependence on the choice of these projections is studied in detail here and a method to overcome this ambiguity in DFT+U, by self-consistently determining the projections, is introduced. The author shows how nonorthogonal representations for electronic states may be used to construct these projections and, furthermore, how DFT+U may be implemented with a linearly increasing cost with respect to system size. The use of nonorthogonal functions in the context of electronic structure calculations is extensively discussed and clarified, with new interpretations and results, and, on this topic.