MAR05-2004-000040

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

**Localization-delocalization transitions in strongly correlated electron systems**

WALTER TEMMERMAN, Daresbury Laboratory, UK

Correlations can give rise to localization of charge and spin of electrons. A methodology will be presented which allows to describe localized states and also localization- delocalization transitions as a function of pressure or doping. The method is the self-interaction- corrected local-spin-density approximation (SIC-LSDA) to density functional theory. The SIC- LSDA can differentiate between localized and itinerant electrons. Results of calculations for 4f, 5f and 3d compounds will illustrate the method.