SIC-LSD study of transition metal valencies in oxide materials

LEON PETIT, Oak Ridge National Laboratory, THOMAS SCHULTHESS, Oak Ridge National Laboratory, AXEL SVANE, Aarhus University, DK, ANDERSON JANOTTI, Oak Ridge National Laboratory, ZDZISLAWA SZOTEK, Daresbury Laboratory, UK, WALTER TEMMERMAN, Daresbury Laboratory, UK — The electronic and magnetic properties of transition metal (TM) oxide materials are largely determined by the degree of localization of the TM d-electrons. With the self-interaction corrected (SIC) local spin density (LSD) approximation, we are able to differentiate between various localization/delocalization scenarios based on total energy considerations, and thus to determine the ground state valency configuration from the global energy minimum. Using the SIC-LSD, we studied the valencies of TM (Co, Mn) impurities in ZnO. We find the position of the TM(0/+ ) donor level to be such that the TM\(^{2+}\) configuration is energetically most favourable both in n-type ZnO, and in ZnO without additional codopants, whilst in p-type ZnO one additional d-electron prefers to delocalize with the resulting TM\(^{3+}\) groundstate configuration. We furthermore investigated the possibility of ferromagnetic order in the corresponding groundstate scenarios. Work supported in part by the Defense Advanced Research Agency and by the Division of Materials Science and Engineering, US Department of Energy. The Oak Ridge National Laboratory is managed by UT-Battelle LLC for the Department of Energy under Contract No. DE-AC05-00OR22725.