Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Hole polaron-polaron interaction in transition metal oxides and its limit to p-type doping[1] SHIYOU CHEN, East China Normal University, and JCAP, Materials Sciences Division, Lawrence Berkeley National Lab, LIN-WANG WANG, JCAP, Materials Sciences Division, Lawrence Berkeley National Lab — Traditionally the origin of the poor p-type conductivity in some transition metal oxides (TMOs) was attributed to the limited hole concentration: the charge-compensating donor defects, such as oxygen vacancies and cation interstitials, can form spontaneously as the Fermi energy shifts down to near the valence band maximum. Besides the thermodynamic limit to the hole concentration, the limit to the hole mobility can be another possible reason, e.g., the hole carrier can form self-trapped polarons with very low carrier mobility. Although isolated hole polarons had been found in some TMOs, the polaron-polaron interaction is not well-studied. Here we show that in TMOs such as TiO_2 and V_2O_5, the hole polarons prefer to bind with each other to form bipolarons, which are more stable than free hole carriers or separated polarons. This pushes the hole states upward into the conduction band and traps the holes. The rise of the Fermi energy suppresses the spontaneous formation of the charge-compensating donor defects, so the conventional mechanism becomes ineffective. Since it can happen in the impurity-free TMO lattices, independent of any extrinsic dopant, it acts as an intrinsic and general limit to the p-type conductivity in these TMOs.

[1]This material is based upon work performed by the JCAP, a US DOE Energy Innovation Hub, the NSFC (No. 61106087 and 91233121) and special funds for major state basic research (No. 2012CB921401).

Shiyou Chen
East China Normal University

Date submitted: 15 Nov 2013 Electronic form version 1.4