Mapping Structural Changes in Electrode Materials: Application of the Hybrid Eigenvector-Following DFT Method to Layered $Li_{0.5}MnO_2$

Ieuan D. Seymour,[†] Sudip Chakraborty,[‡] Derek S. Middlemiss,[§] David J. Wales[†] and Clare P. Grey[†] *

Supporting Information

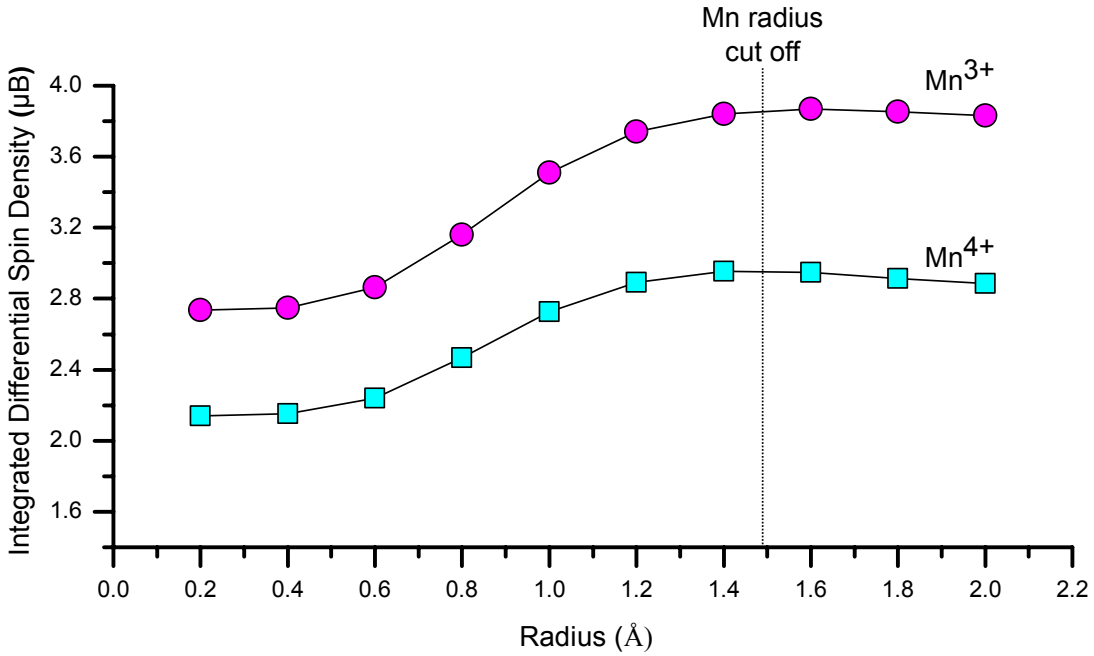

Figure S1: Variation in the integrated differential spin density of electrons as a function of sphere radius around the Mn centres in a primitive cell of $Li_{0.5}MnO_2$ containing one Mn^{3+} ion and one Mn^{4+} ion.

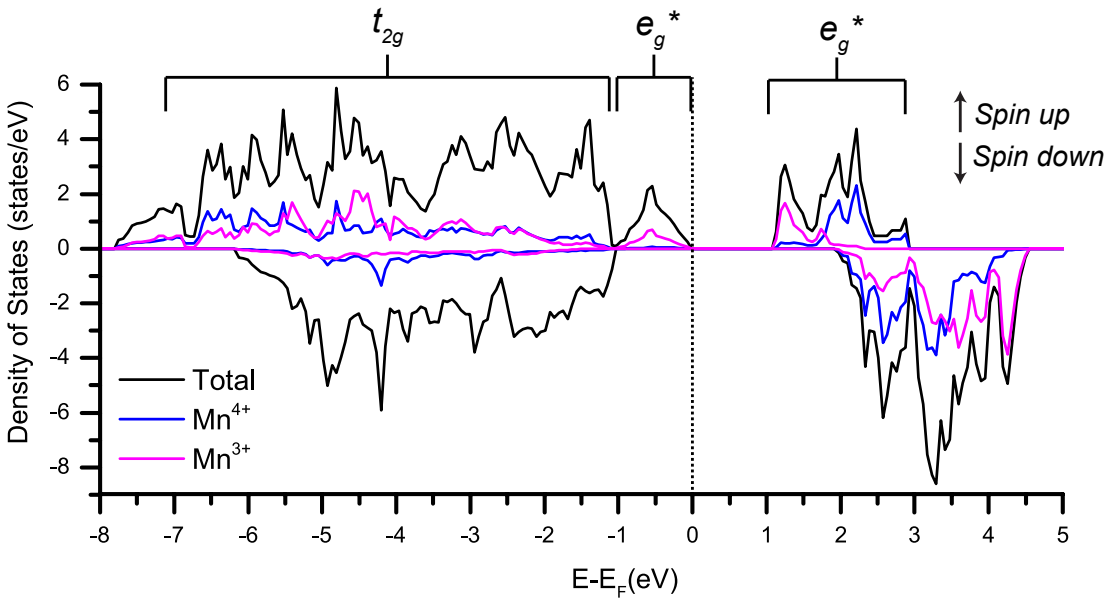

Figure S2: Density of states plot for $Li_{0.5}MnO_2$ with Li vacancy chain configuration. Total density of states shown in black, with partial Mn^{3+} and Mn^{4+} density of states shown in purple and blue respectively. The Fermi level is indicated with a dashed line.

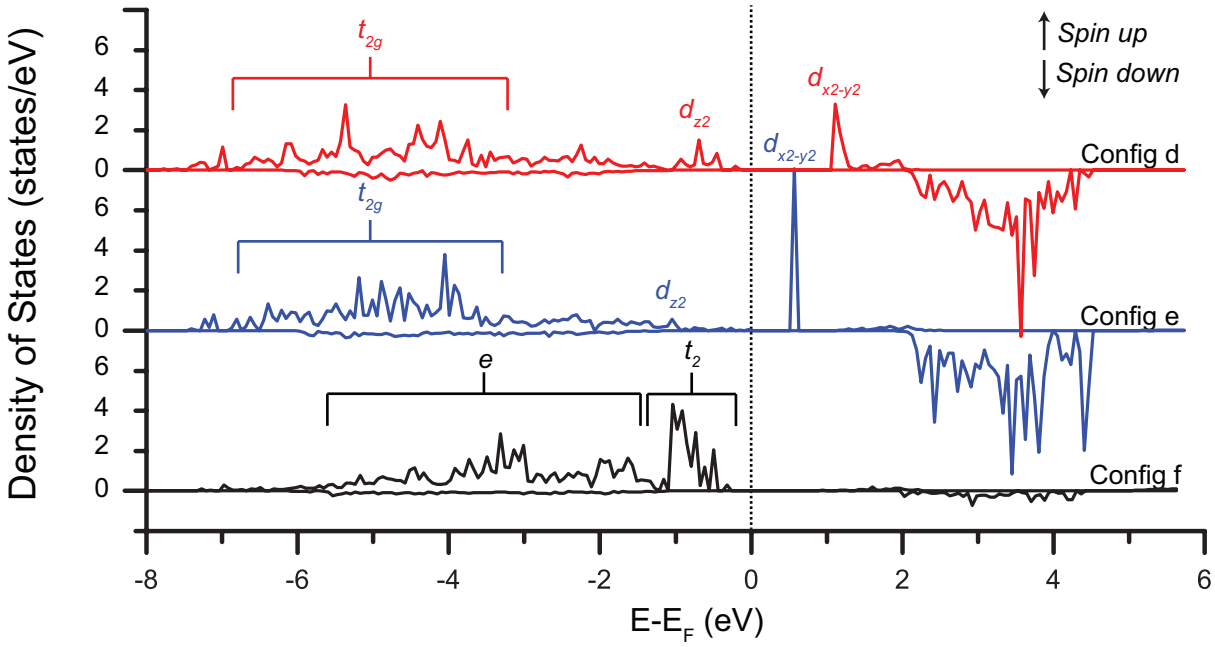

Figure S3: Projected density of states plot for diffusing Mn in local minima of $Li_{0.5}MnO_2$ 2x2x2 supercell. Top: (configuration d) Mn in octahedral site. Middle: (configuration e) Mn in square pyramidal MnO_5 configuration. Bottom: (configuration f) Mn in tetrahedral sites forming Mn-Li 'dumbbell' structure. The Fermi level is indicated with a dashed line.

[†]Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK.
[‡]Department of Physics and Astronomy, Uppsala University, Uppsala, SE 75120, Sweden.
[§] Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK.