Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information

Understanding the origin of high-rate intercalation pseudocapacitance in Nb_2O_5 crystals

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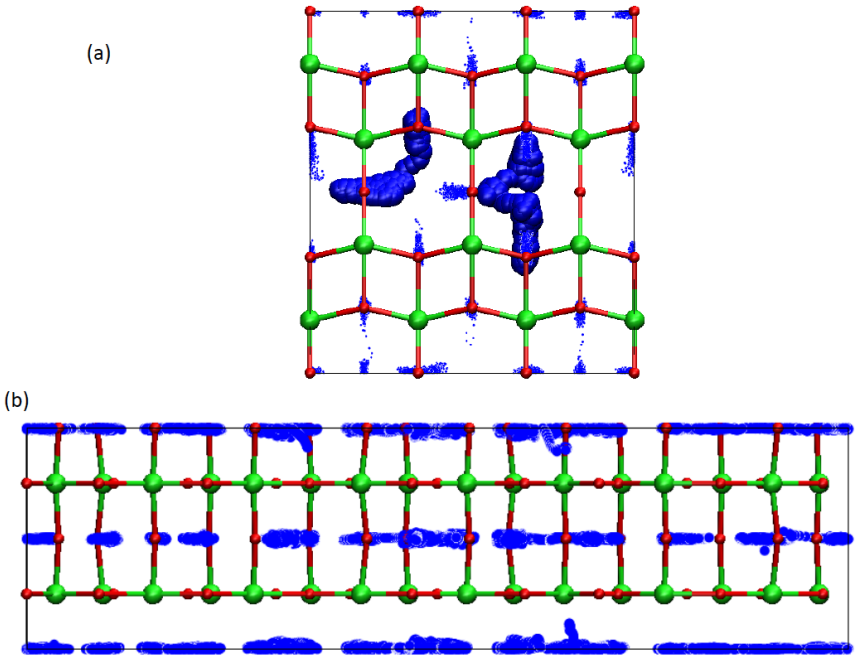

FIGURE S1: (a) Overlapping trajectories from a T=300K run for *m*-Nb_2O_5. Two specific Li-atoms are drawn as large spheres to explicitly show their diffusive path in the crystal structure (b) Overlapping trajectories in the *o*-Nb_2O_5 at T=600K at a different orientation show how the lithium motion is confined to the 2D oxygen plane without the niobium atoms.

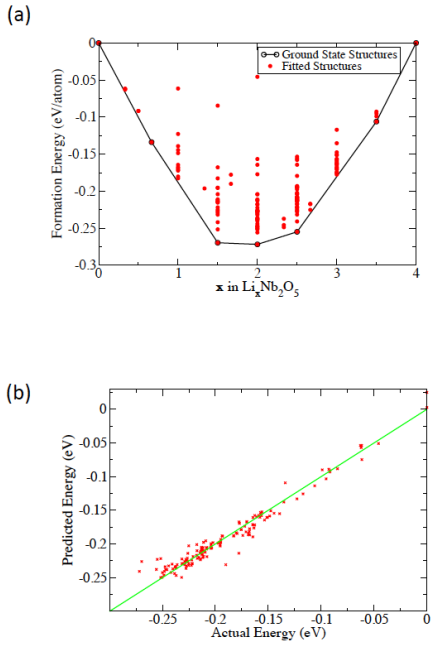

FIGURE S2: (a) formation energy and (b) goodness of fit for the cluster expansion Hamiltonian of $Li_xNb_2O_5$ in the *m*-Nb_2O_5 host structure.

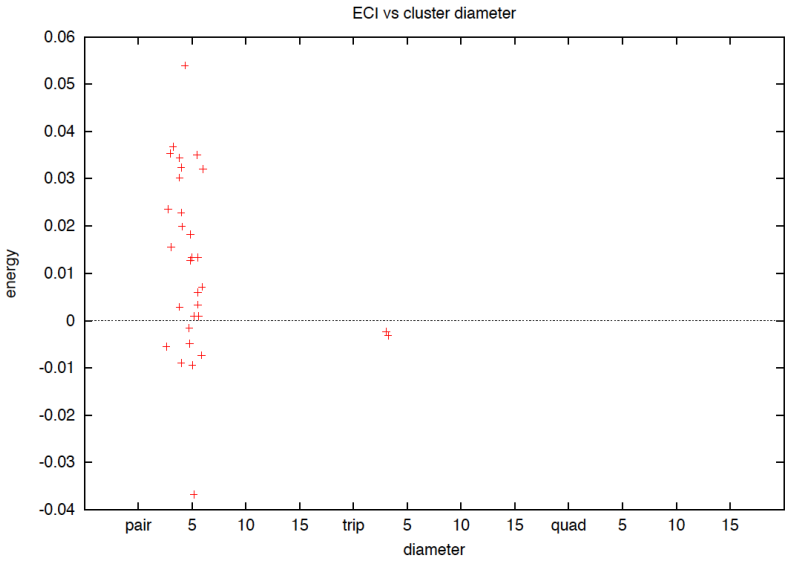

FIGURE S3: Effective cluster interactions are plotted for the *m*-phase and shows convergence with cluster diameter.