Supporting Information

Understanding the origin of high-rate intercalation pseudocapacitance in Nb$_2$O$_5$ crystals

Andrew A. Lubimtsev$^{1,2}$, Paul R. C. Kent$^{1,4}$, B. G. Sumpter$^1$ and P. Ganesh$^1$*

$^1$Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TN 37830

$^2$Department of Engineering Science and Mechanics, Pennsylvania State University, University Park, PA 16802

$^4$Computer Science and Mathematics Division, Oak Ridge National Laboratory, TN 37830
FIGURE S1: (a) Overlapping trajectories from a T=300K run for m-Nb$_2$O$_5$. 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$_2$O$_5$ 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$_x$Nb$_2$O$_5$ in the $m$-Nb$_2$O$_5$ host structure.

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