Supporting Information

**Theoretical Design of MoO$_3$-Based High-Rate Lithium Ion Battery Electrodes: The Importance/Effect of Dimensionality Reduction**

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Figure S1. Band structures of MoO$_3$ pristine (a) and Li-adsorbed (b) $12c$ NRs, pristine (c) and Li-adsorbed (d) $11a$ NRs.

Figure S2. Top view of Li diffusion $T_{O3H}$ and $T_{O2O1}$ pathways on $12c$ MoO$_3$ NR along the transverse direction. The numbers indicate the diffusion barriers in eV. The cyan (light cyan) and red (light red) balls denote Mo and atoms of one (the other) sublayer, respectively.
**Figure S3.** Top view of Li diffusion pathways $T_{01H}$ and $T_{03O2}$ on 12-c MoO$_3$ NR along the transverse direction. The numbers indicate the diffusion barriers in eV. The cyan (light cyan) and red (light red) balls denote Mo and atoms of one (the other) sublayer, respectively.

**Figure S4.** Top (a) and bottom (b) views of Li diffusion pathways $T_{02O3}$ and $T_{02E7}$ on 11-a MoO$_3$ NR along the transverse direction. The numbers indicate the diffusion barriers in eV. The cyan (light cyan) and red (light red) balls denote Mo and atoms of one (the other) sublayer, respectively.