Supporting Information

Theoretical Design of MoO_3-Based High-Rate Lithium Ion Battery Electrodes: The Importance/Effect of Dimensionality Reduction

Fengyu Li,[†] Zhongfang Chen[†,*]

Department of Physics, Department of Chemistry, Institute for Functional Nanomaterials, University of Puerto Rico, Rio Piedras Campus, San Juan, PR 00931.

* To whom correspondence should be addressed. Email: zhongfangchen@gmail.com (Z.C.)

[†] University of Puerto Rico

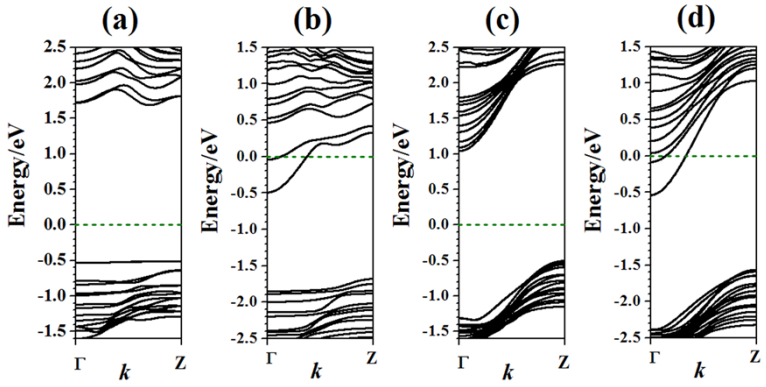

Figure S1. Band structures of MoO_3 pristine (a) and Li-adsorbed (b) *12-c* NRs, pristine (c) and Li-adsorbed (d) *11-a* NRs.

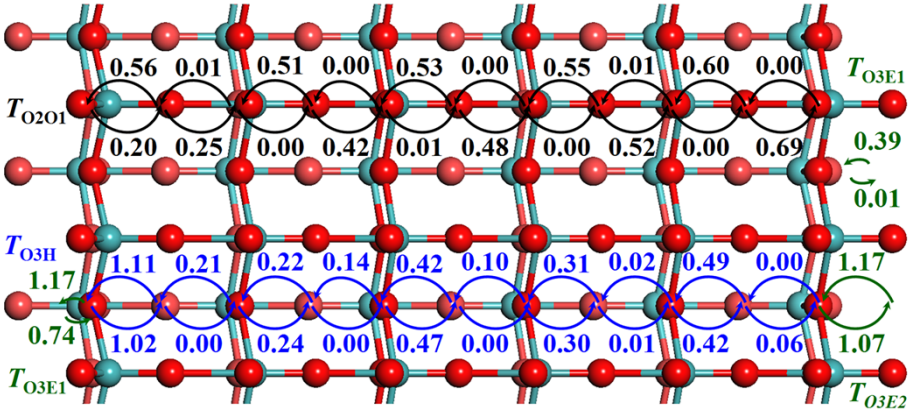

Figure S2. Top view of Li diffusion T_{O3H} and T_{O2O1} pathways on *12-c* MoO_3 NR along the transverse direction. The numbers indicate the diffusion barriers in eV. The cyan (light cyan) and red (light red) balls denote Mo and atoms of one (the other) sublayer, respectively.

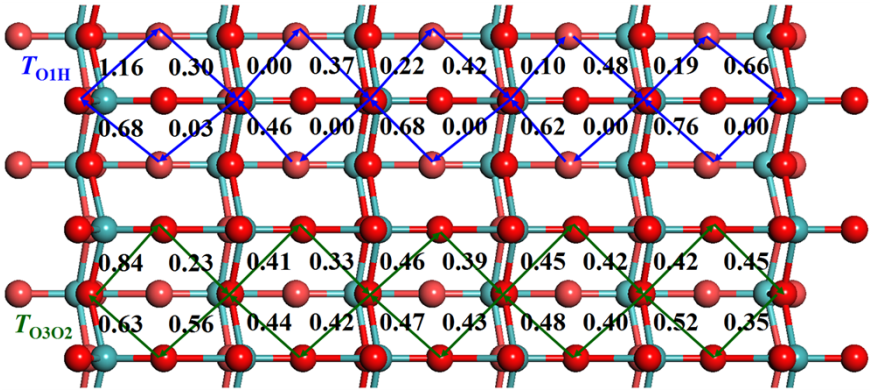

Figure S3. Top view of Li diffusion pathways T_{O1H} and T_{O3O2} on *12-c* MoO_3 NR along the transverse direction. The numbers indicate the diffusion barriers in eV. The cyan (light cyan) and red (light red) balls denote Mo and atoms of one (the other) sublayer, respectively.

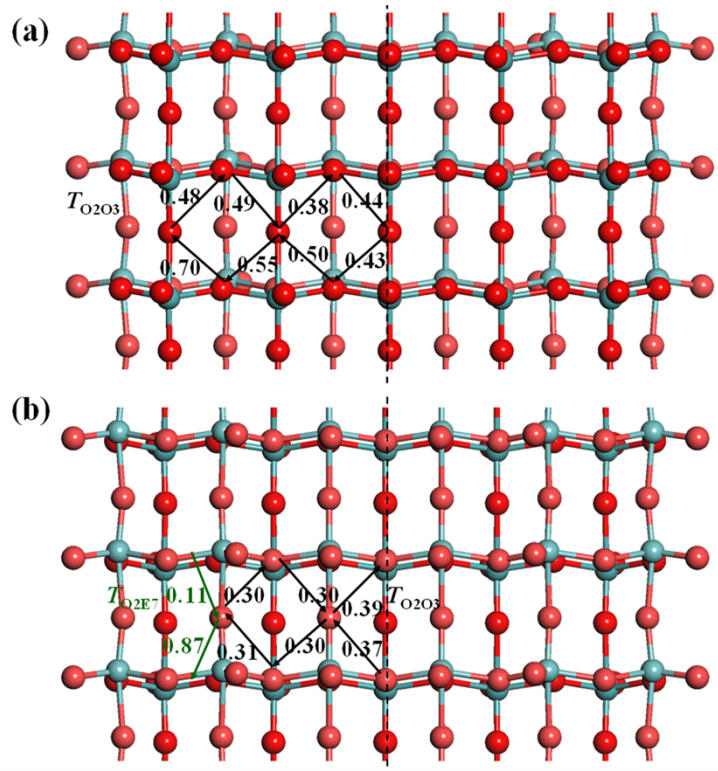

Figure S4. Top (a) and bottom (b) views of Li diffusion pathways T_{O2O3} and T_{O2E7} on *11-a* MoO_3 NR along the transverse direction. The numbers indicate the diffusion barriers in eV. The cyan (light cyan) and red (light red) balls denote Mo and atoms of one (the other) sublayer, respectively.