Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

"Super-alkalis as Building Blocks of One-Dimensional Hierarchical Electride"

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Figure S1. (a) Optimized structure of Li_3O cluster in a planar configuration. (b) Molecular dynamics simulation at 300 K for a perovskite structure Li_3OGeI_3, where Li_3O clusters are serving as cations. The clusters self-assemble into chain structures.

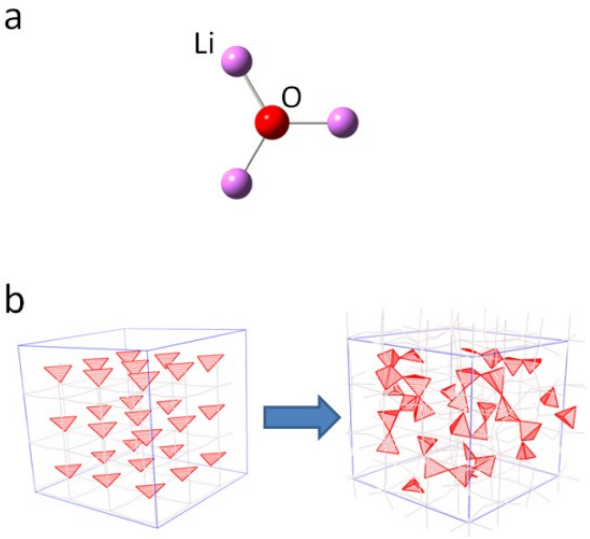

Figure S2. Optimized structure of three-dimensional Li_3O assuming it has the same crystal structure as Cs_3O.

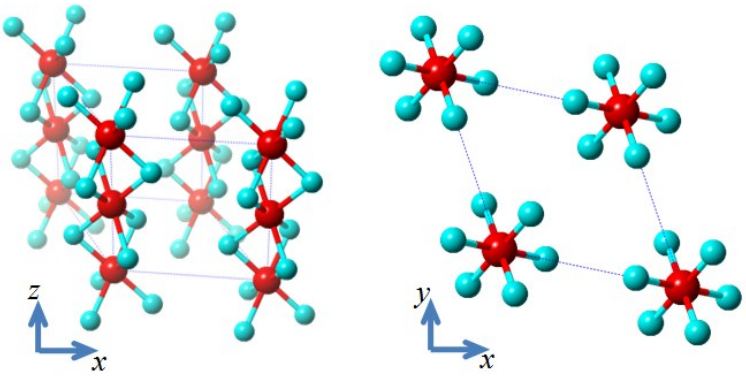

Figure S3. Calculated Li-O phase diagram, where Li_3O is found to be above the convex hull.

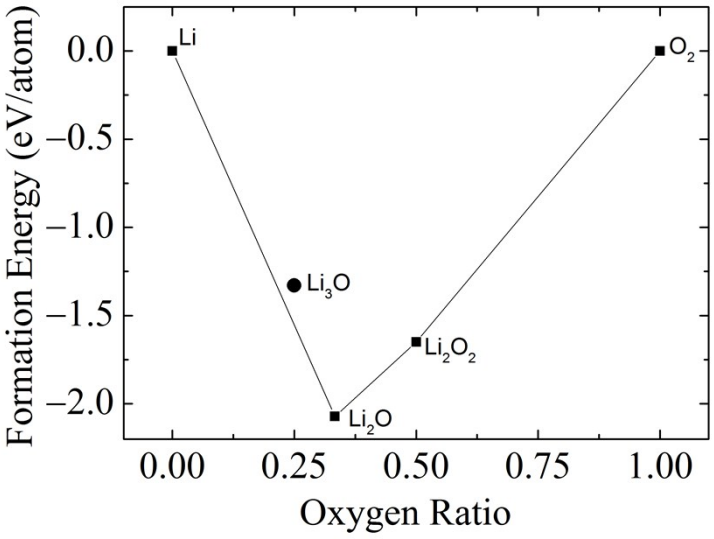

Figure S4. The snapshot of 1D 1×1×6 Li_3O after simulations at 300 for 5 ps. The structure remains stable.

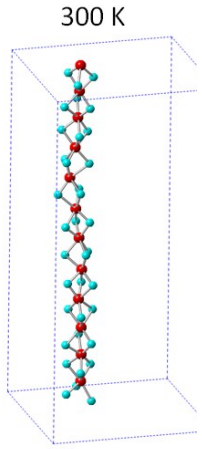

Figure S5. Calculated work functions of Li_3O and Li_3O@BNNT. The Fermi energies for the two are −2.36 and −1.51 eV, respectively.

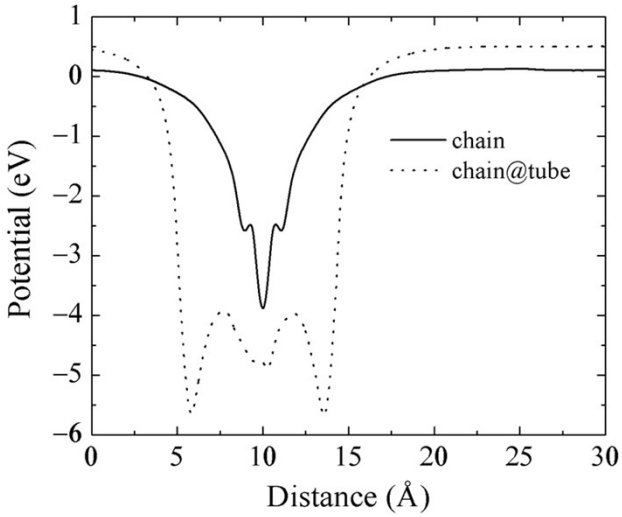

Figure S6. Optimized structure of the unit cell of Li_3O@BNNT activating four CO_2 molecules at once.