Supporting Information

Robust Topological States in Bi$_2$Se$_3$ Against Surface Oxidation

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Figure S1. Top and side views of (a) one O atom oxidized ($O^{\frac{1}{2}}_{Se} - 2*2$ supercell), (b) two O atoms oxidized ($O^{\frac{2}{2}}_{Se} - 2*2$ supercell), (c) three O atoms oxidized ($O^{\frac{3}{2}}_{Se} - 2*2$ supercell), and four O atoms oxidized ($O^{\frac{4}{2}}_{Se} - 2*2$ supercell) on Se-terminated Bi$_2$Se$_3$ slab with (2×2) supercell surface. The corresponding adsorption energies for per O atom are also listed.
Figure S2. Electronic band structures of surface oxidization for Se-terminated Bi$_2$Se$_3$ slabs with (2×2) supercell surface: (a) $O_{3e}^1$-2*2supercell, (b) $O_{3e}^2$-2*2supercell, (c) $O_{3e}^3$-2*2supercell, and (d) $O_{3e}^4$-2*2supercell.
Figure S3. Top and side views of (a) pristine, (b) one O atom oxidized \( \text{O}^1_{\text{Bi}} \), and (c) two O atoms oxidized \( \text{O}^2_{\text{Bi}} \) on Bi-terminated Bi\(_2\)Se\(_3\) slab with \((1\times1)\) cell surface. The adsorption energies for per O atom of \( \text{O}^1_{\text{Bi}} \) and \( \text{O}^2_{\text{Bi}} \) are -2.449 eV and -1.489 eV, respectively.
Figure S4. Structure diagrams of oxidized Bi$_2$Se$_3$ slab with different oxygen concentrations and oxidation depths along the normal direction of the surface: (a) Bi$_{20}$Se$_{30}$O$_{4}$, (b) Bi$_{20}$Se$_{30}$O$_{6}$, (c) Bi$_{20}$Se$_{30}$O$_{8}$, and (d) Bi$_{20}$Se$_{30}$O$_{10}$. 