Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Strain-Tunable Electronic Properties and Lithium Storage of 2D Transition Metal Carbide (MXene) Ti_2CO_2 as Flexible Electrodes

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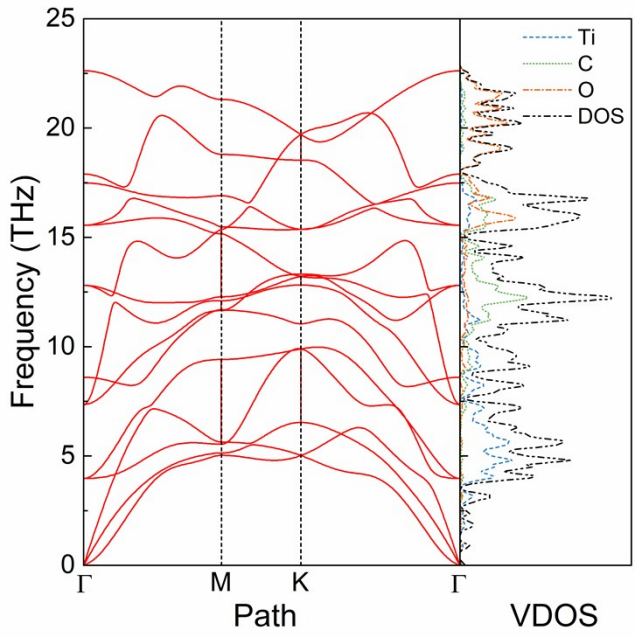

Figure S1. Phonon dispersion and total and projected vibrational density of states (VDOS) for pristine Ti_2CO_2.

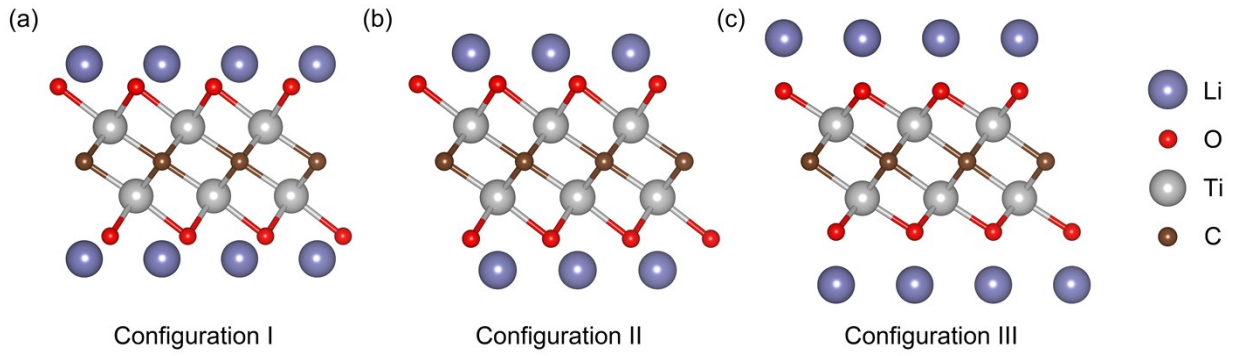

Figure S2. Possible configurations I, II, III for the first Li adsorption layer.

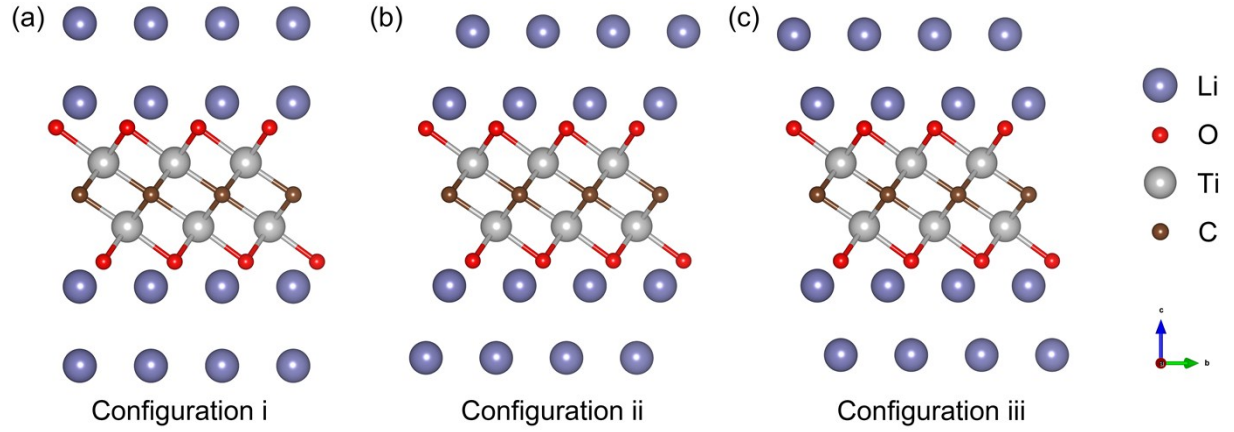

Figure S3. Possible configurations I, II, III for the second Li adsorption layer.

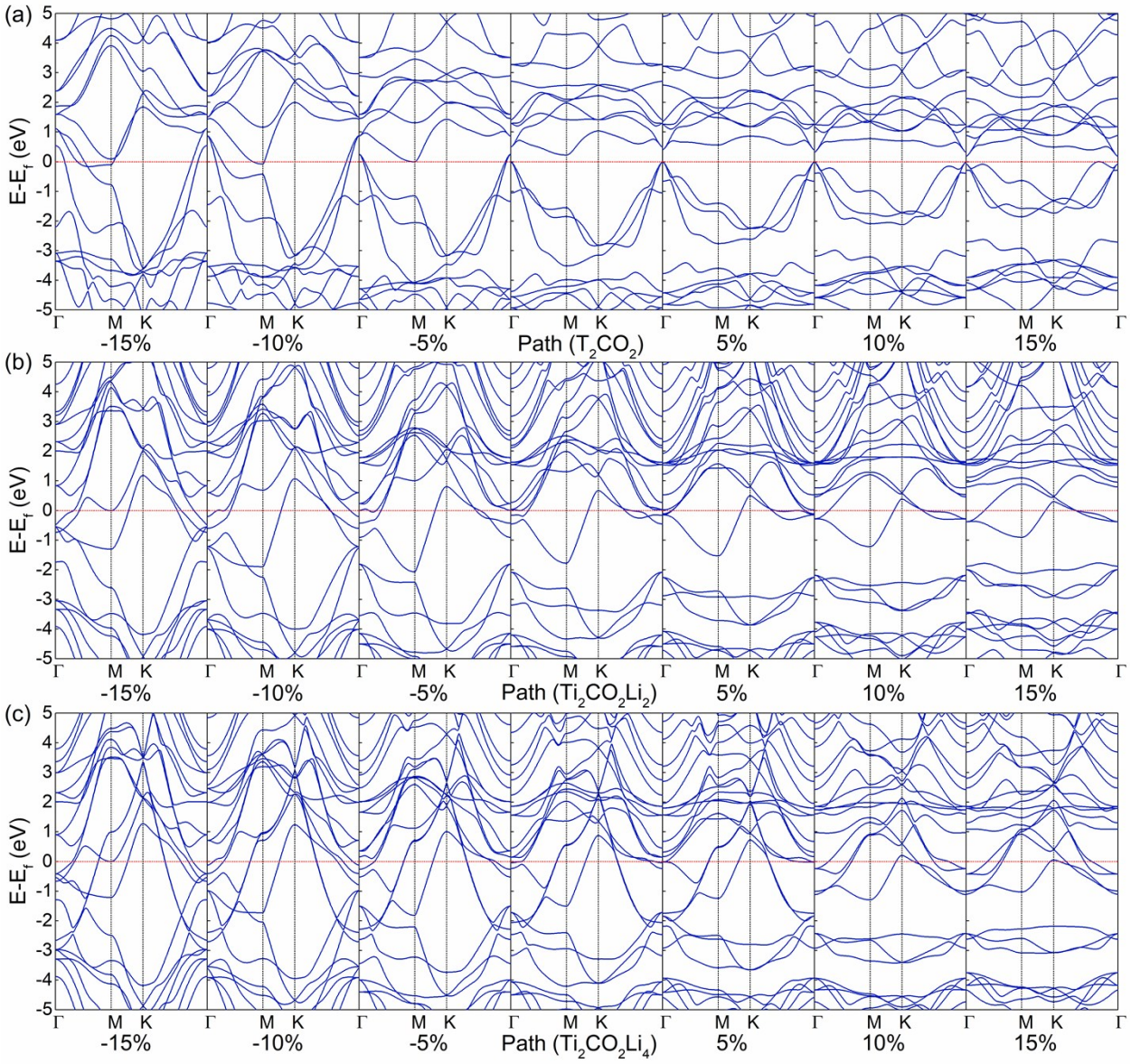

Figure S4. Electronic band structures of (a) Ti_2CO_2, (b) $Ti_2CO_2Li_2$ and (c) $Ti_2CO_2Li_4$ under biaxial strains from –15% to +15% with step size of 5%. Here Fermi energy levels have been chosen as zero energy references.

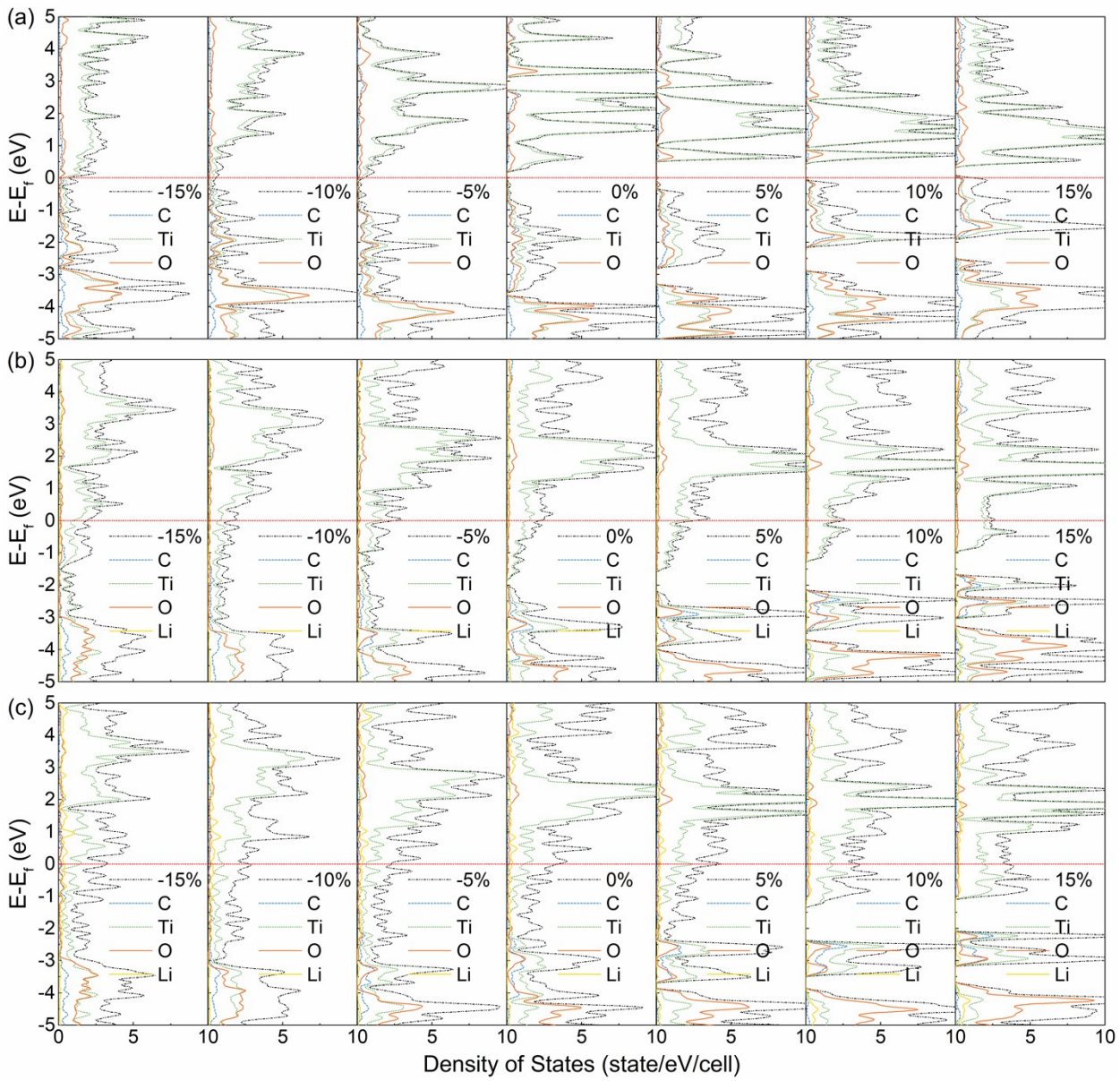

Figure S5. Total and partial density of states (DOS) for (a) Ti_2CO_2, (b) $Ti_2CO_2Li_2$ and (c) $Ti_2CO_2Li_4$ under biaxial strains from –15% to +15% with step size of 5%. Here Fermi energy levels have been chosen as zero energy references.

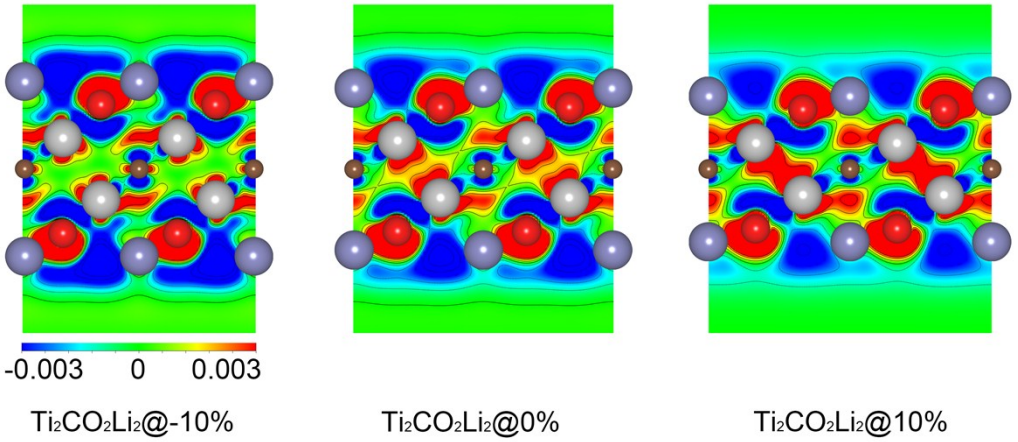

Figure S6. Electron density differences projected on (110) planes after single layer Li adsorption for $Ti_2CO_2Li_2$ at strain of −10%, 0% and 10%, respectively. The unit of color bar is e/Å^3.

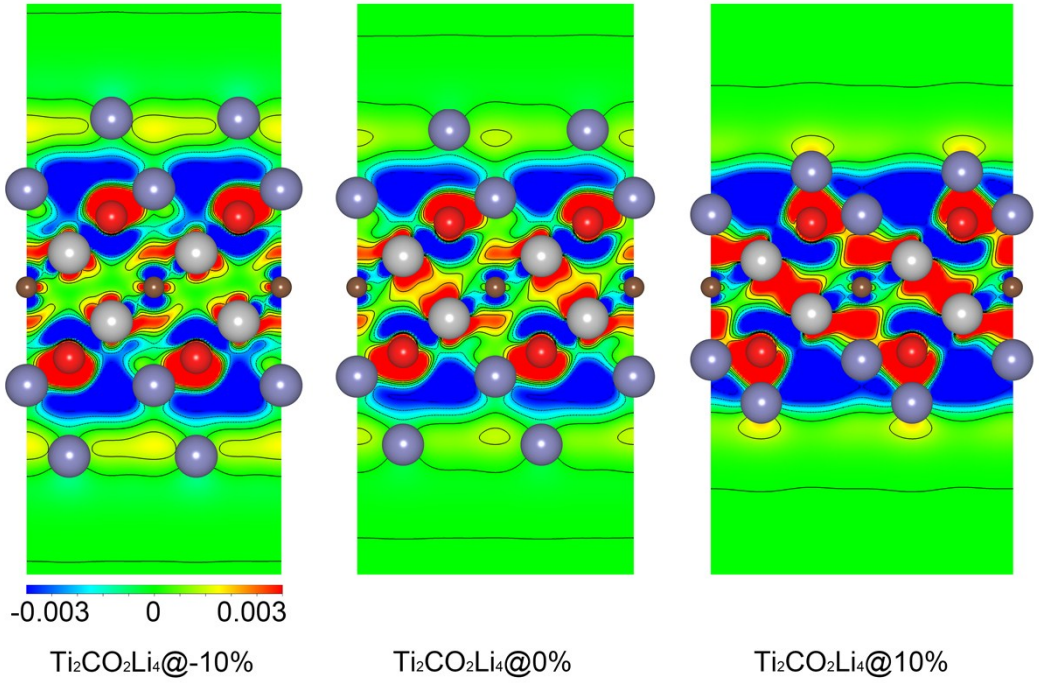

Figure S7. Electron density differences projected on (110) planes after double layer Li adsorption for $Ti_2CO_2Li_4$ at strain of −10%, 0% and 10%, respectively. The unit of color bar is e/Å^3.

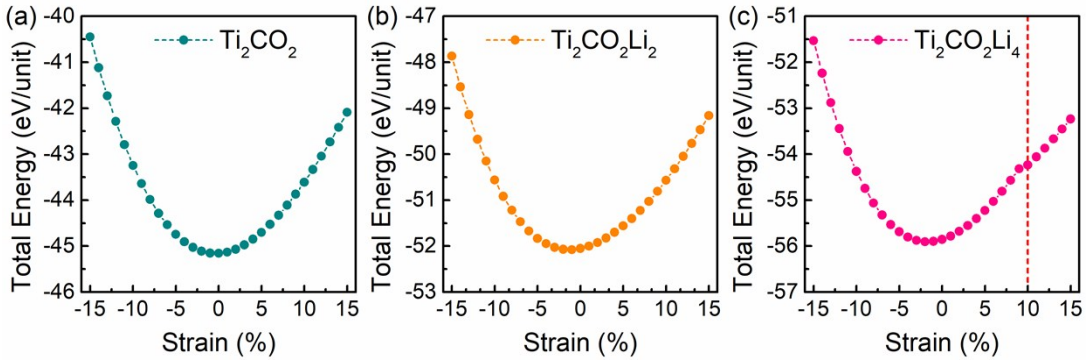

Figure S8. (a-c) Strain dependence of total energies for Ti_2CO_2, $Ti_2CO_2Li_2$ and $Ti_2CO_2Li_4$.