Supporting Information

STRUCTURAL AND ELECTRONIC PROPERTIES OF LITHIATED SnO_2. A PERIODIC DFT STUDY

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Table S1. Intercalation sites (fractional coordinates) considered for lithium intercalation and calculated cohesive energies (in eV) for all Li_xSnO_2 systems

X	Model	Intercalation sites for Li_xSnO_2 periodic models								E_{coh}
0										283.2
1/16	1/16A	(0 ¼ ¾)								286.4
1/8	1/8A	(0 ¼ ¼)	(0 ¼ ¾)							288.7
	1/8B	(0 ¼ ¾)	(0 ¾ ¾)							288.8
	1/8C	(0 ¾ ¾)	(½ ¾ ¾)							288.5
	1/8D	(0 ¼ ¼)	(½ ¼ ¾)							288.1
	1/8E	(0 ¼ ¾)	(½ ¾ ¾)							287.7
	1/8F	(0 ¼ ¾)	(½ ¾ ¼)							287.6
	1/8G	(0 ¼ ¾)	(¼ ½ ¾)							288.4
	1/8H	(0 ¼ ¾)	(¼ ½ ¼)							288.6
1/4	1/4A	(0 ¼ ¼)	(0 ¼ ¾)	(½ ¼ ¼)	(½ ¼ ¾)					293.6
	1/4B	(0 ¾ ¼)	(½ ¼ ¾)	(½ ¼ ¼)	(½ ¼ ¾)					292.9
	1/4C	(0 ¼ ¾)	(0 ¾ ¾)	(½ ¼ ¾)	(½ ¾ ¾)					292.8
	1/4D	(0 ¼ ¾)	(0 ¾ ¾)	(½ ¼ ¼)	(½ ¾ ¼)					293.8
	1/4E	(0 ¼ ¾)	(½ ¼ ¾)	(½ ¼ ¼)	(½ ¾ ¾)					294.0
	1/4F	(0 ¼ ¾)	(½ ¼ ¾)	(½ ¼ ¾)	(½ ¾ ¼)					294.3
	1/4G	(0 ¼ ¾)	(½ ¼ ¾)	(¼ ½ ¾)	(¾ ½ ¼)					294.0
	1/4H	(0 ¼ ¾)	(½ ¼ ¾)	(¼ ½ ¾)	(¾ ½ ¾)					293.4
1/2	1/2A	(0 ¼ ¼)	(0 ¼ ¾)	(½ ¼ ¼)	(½ ¼ ¾)	(½ ¼ ¼)	(½ ¼ ¾)	(½ ¾ ¼)	(½ ¾ ¾)	303.4
	1/2B	(0 ¼ ¼)	(½ ¼ ¾)	(½ ¼ ¾)	(½ ¾ ¼)	(¼ 0 ¼)	(¼ ½ ¾)	(¾ 0 ¾)	(¾ ½ ¼)	305.0
	1/2C	(0 ¼ ¾)	(½ ¼ ¾)	(½ ¼ ¾)	(½ ¾ ¾)	(¼ 0 ¾)	(¼ ½ ¾)	(¾ 0 ¾)	(¾½ ¾)	301.2
	1	(0 ¼ ¼) (¼ 0 0)	(0 ¼ ¾) (¼ 0 ½)	(½ ¼ ¼) (¼ ½ 0)	(½ ¼ ¾) (¼ ½ ¾)	(½ ¼ ¼) (¾ 0 0)	(½ ¼ ¾) (¾ 0 ½)	(½ ¾ ¼) (¾ ½ 0)	(½ ¾ ¾) (¾ ½ ½)	325.1

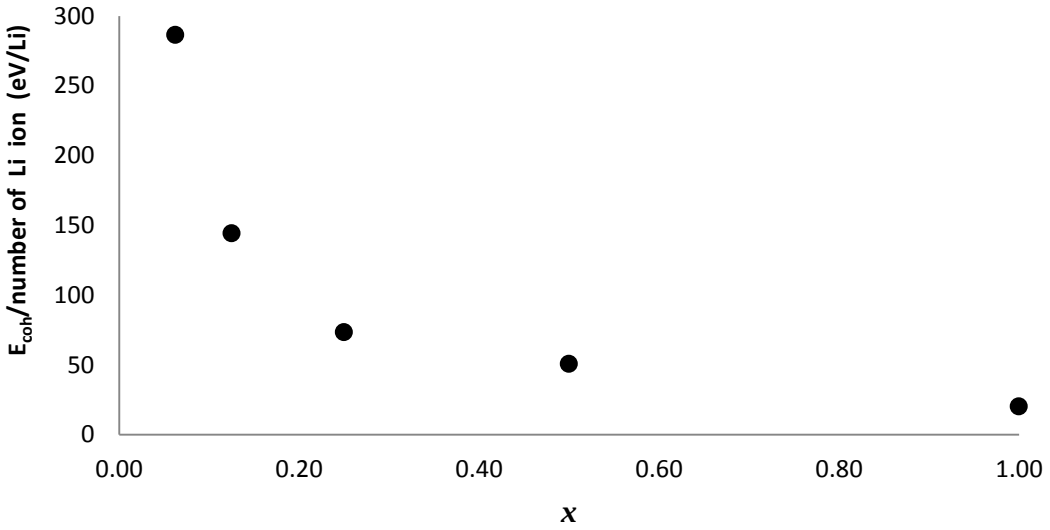

Figure S1. Cohesive energies per number of intercalated Li ions in the 2×2×2 supercell.

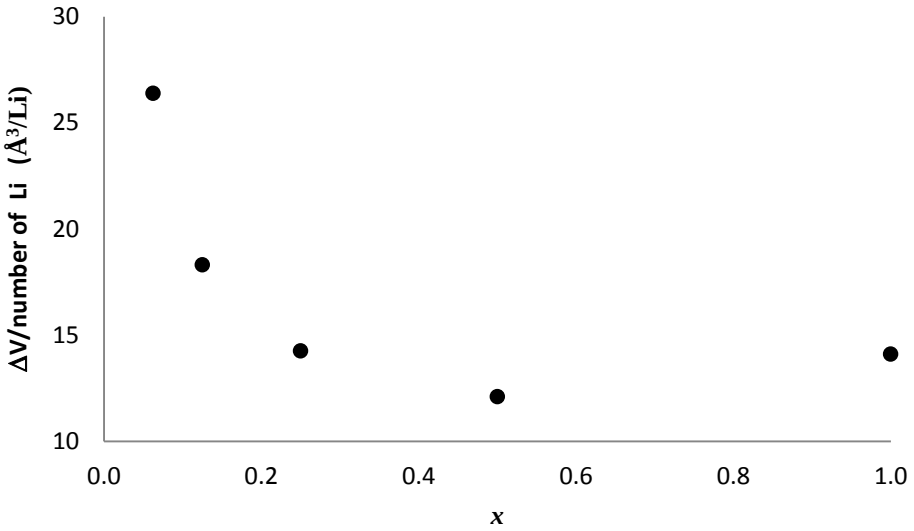

Figure S2. Variation in volume per lithium atom in the 2×2×2 supercell.

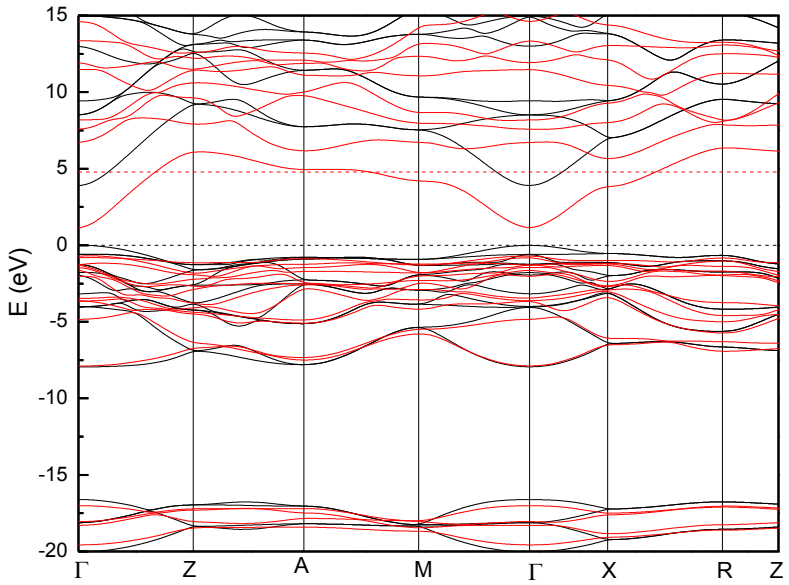

Figure S3. Calculated electronic band structure diagrams for pure SnO_2 (black line), $Li_{0.5}SnO_2$ (red line). The dashed lines refer to the corresponding Fermi level.

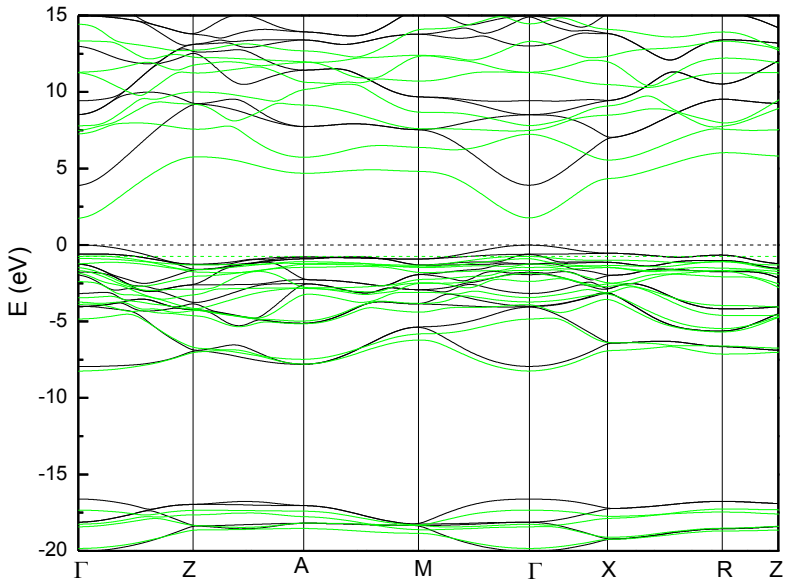

Figure S4. Calculated electronic band structure diagrams for pure SnO_2 (black line) and Li_0SnO_2 (green line). The dashed lines refer to the corresponding Fermi level.

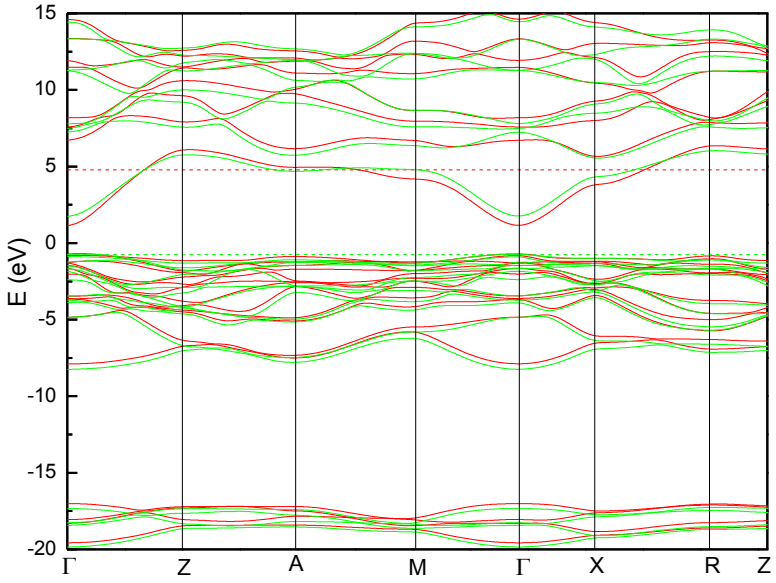

Figure S5. Calculated electronic band structure diagrams for $Li_{0.5}SnO_2$ (red line) and Li_0SnO_2 (green line). The dashed lines refer to the corresponding Fermi level.

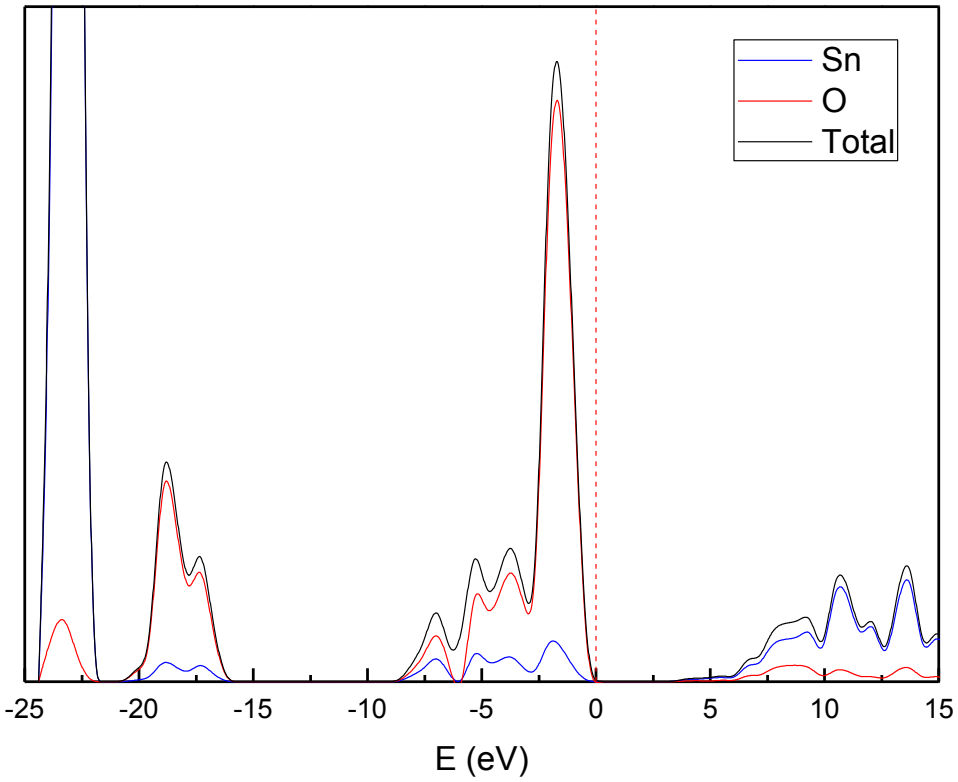

Figure S6. Calculated DOS and PDOS of pure SnO_2. The dashed lines refer to the Fermi level. The bands centered about -23 eV and -19 eV correspond to tin 4*d*-like (VB3) and O 2*s*-like (VB2) states, respectively. See text for a detailed description of VB1 and CB.

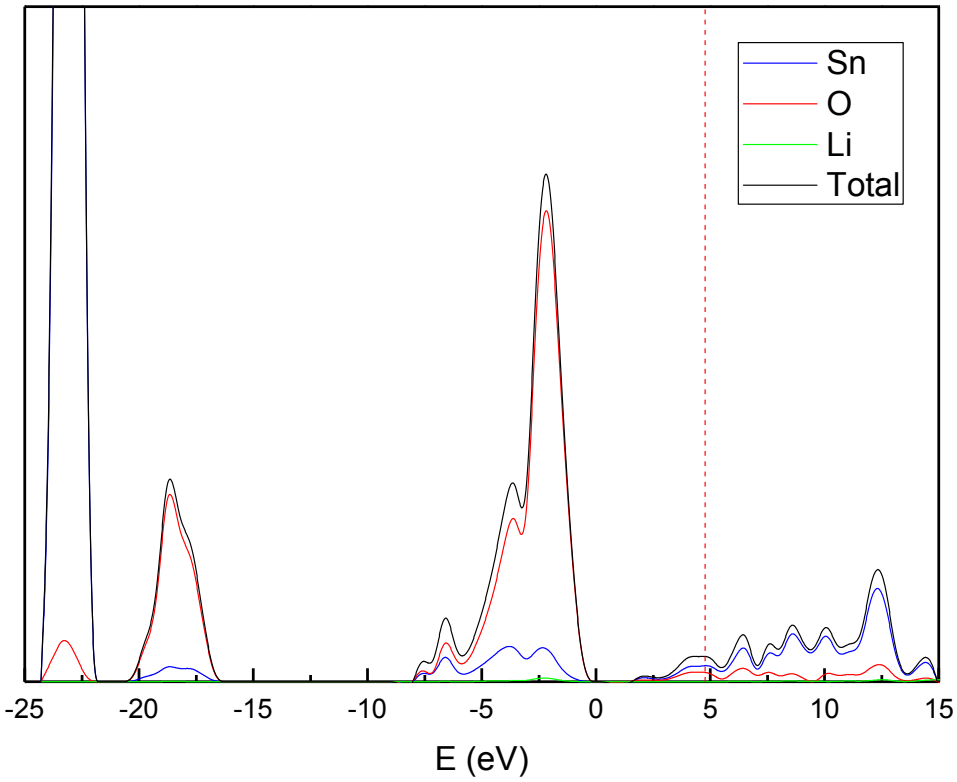

Figure S7. Calculated DOS and PDOS of $Li_{0.5}SnO_2$. The dashed lines refer to the Fermi level.

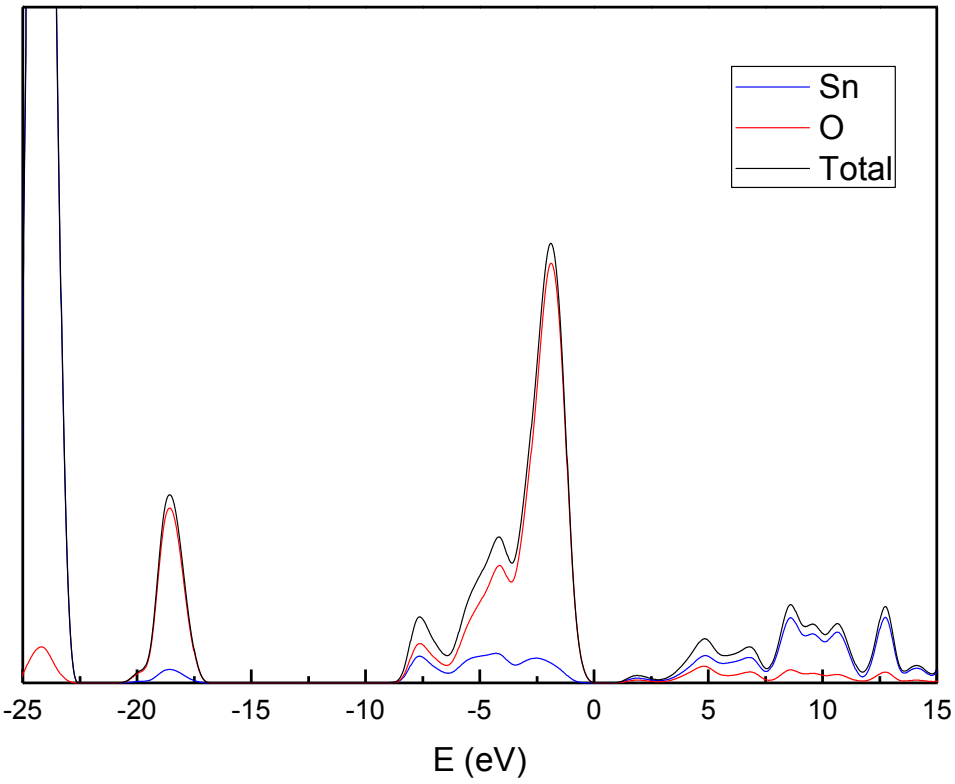

Figure S8. Calculated DOS and PDOS of delithiated Li_0SnO_2 (Li_0SnO_2 which is similar to $Li_{0.5}SnO_2$ where Li ions have been removed without relaxing the lattice).