Supporting Information for:

An ab initio study of TiS_3: a promising electrode material for rechargeable Li and Na ion batteries

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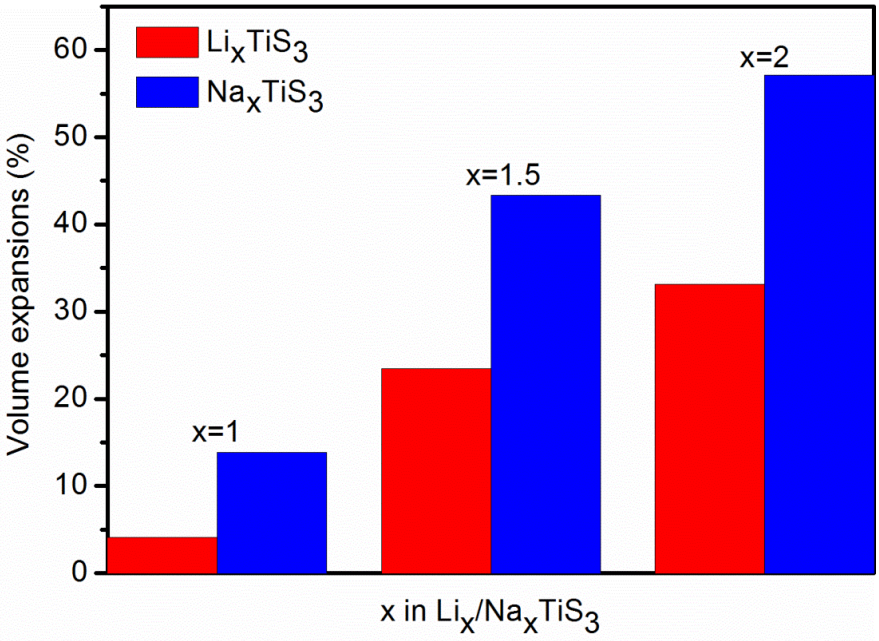

Fig. S1: Volume expansions computed upon Li and Na insertion in bulk TiS_3 (Li_x/Na_xTiS_3) for x=1,1.5 and 2, respectively.

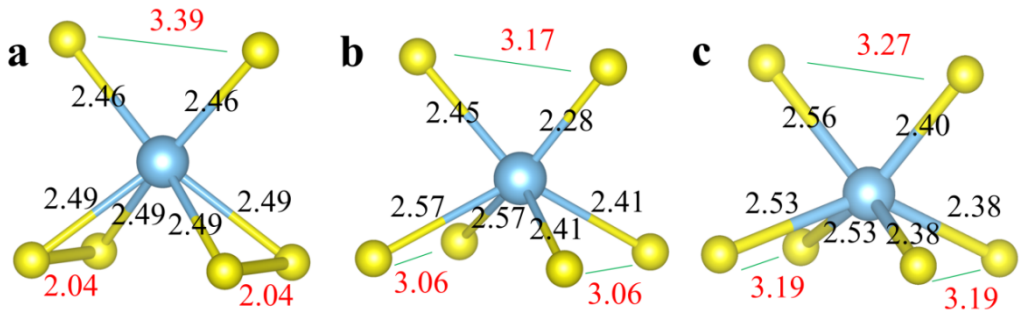

Fig. S2: Bond length of Ti atom and its neighbor sulfur atoms in bulk TiS_3, Li_2TiS_3 and Na_2TiS_3, respectively.

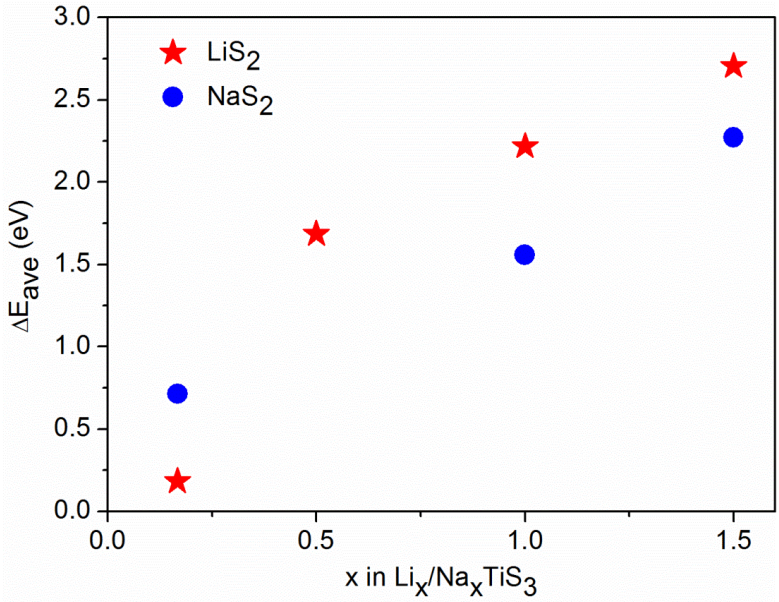

Fig. S3: Reaction trend of average energy difference (ΔE_{ave}) of Li_2S and Na_2S in monolayer Li_x/Na_xTiS_3, respectively.

Table. S1 Energy barriers (∇E) for Li and Na diffusion in bulk and monolayer TiS_3 (eV) with Li/Na atoms absorbed the whole H sites except an unoccupied H site, respectively.

∇E	Monolayer		Bulk	
	Li	Na	Li	Na
H-T_1-H	0.51	0.64	0.57	0.46
H-T_2-H	0.57	0.64	1.61	1.69