

Supplementary material

Journal of Solid State Electrochemistry

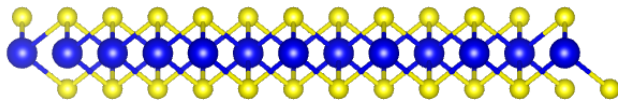
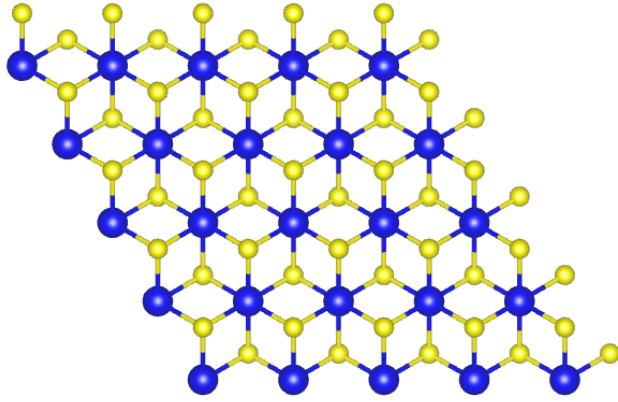
Enhancement of electrochemical performance of monolayer SnS₂ for Li/Na-ion batteries through a sulphur vacancy: A DFT study

C.A. Bekeur¹, R.E. Mapasha^{1*}

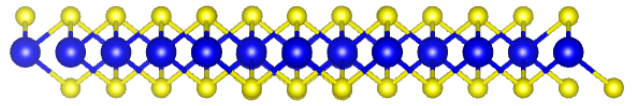
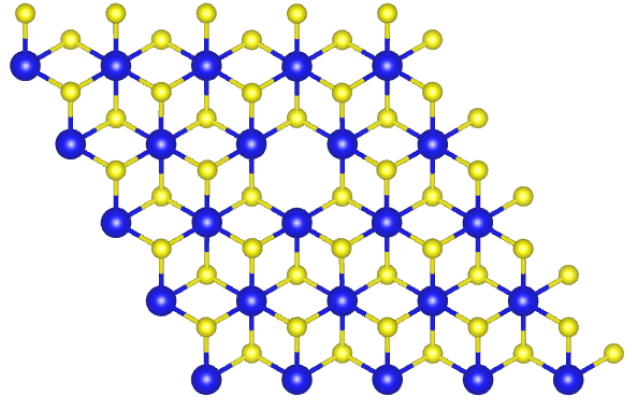
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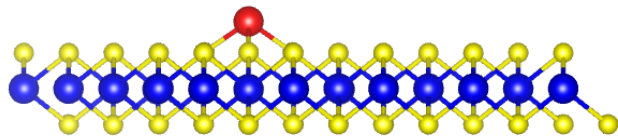
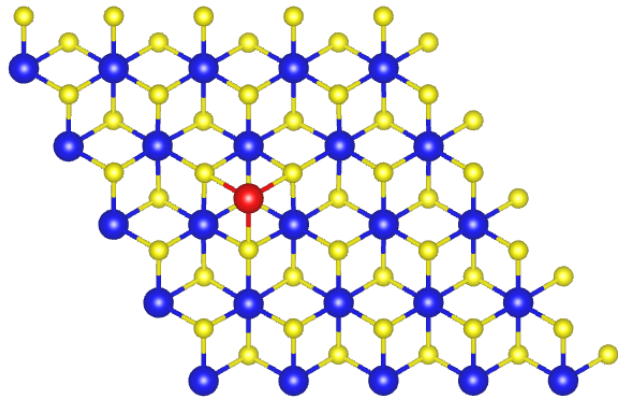
Email: edwin.mapasha@up.ac.za



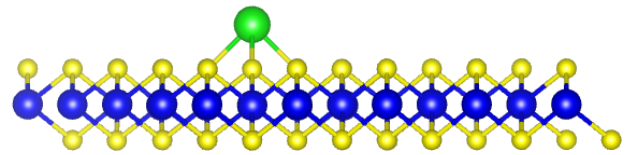
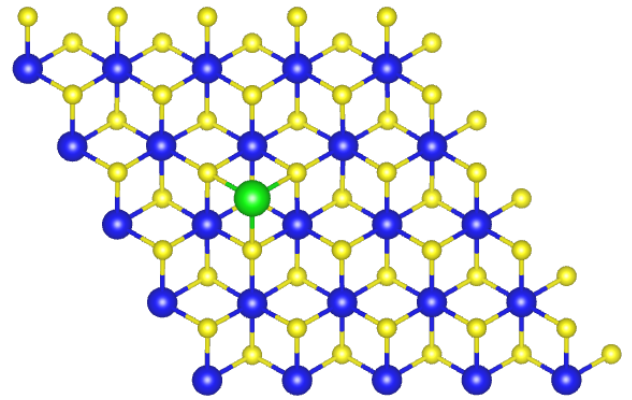
(a) Pristine SnS_2



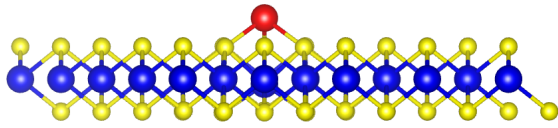
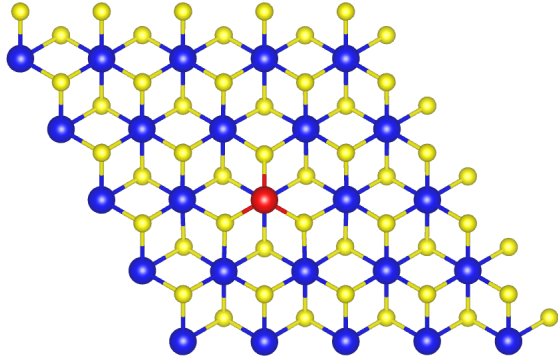
(b) SnS_2 with S-vacancy



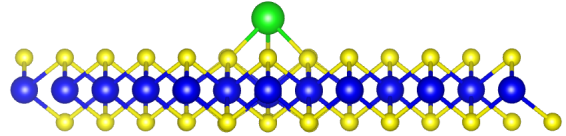
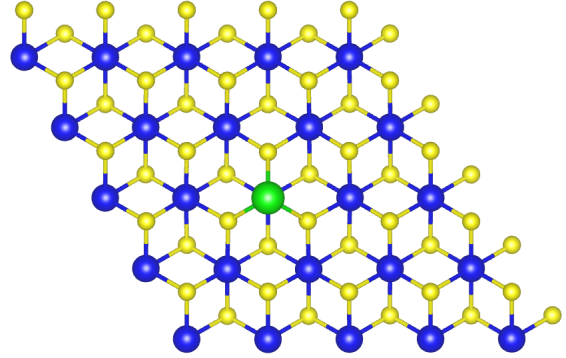
(c) Li at H_{SnS_2} site on pristine SnS_2



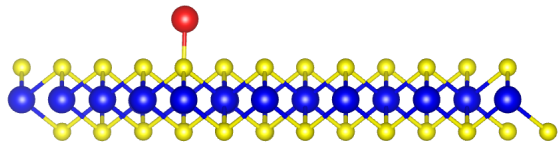
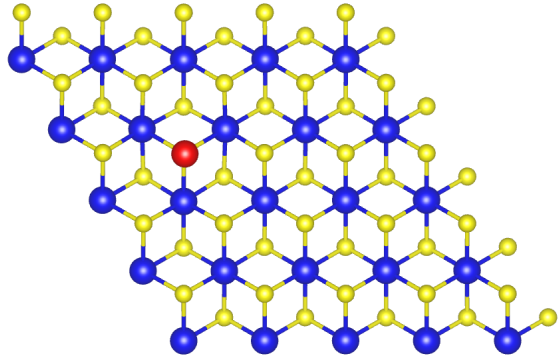
(d) Na at H_{SnS_2} site on pristine SnS_2



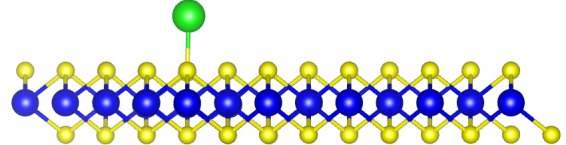
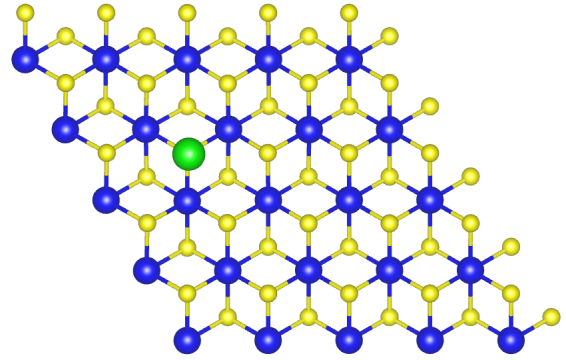
(e) Li at T_{Sn} site on pristine SnS_2



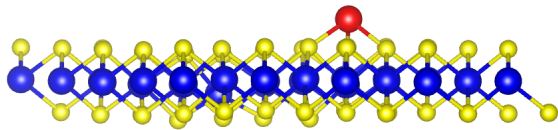
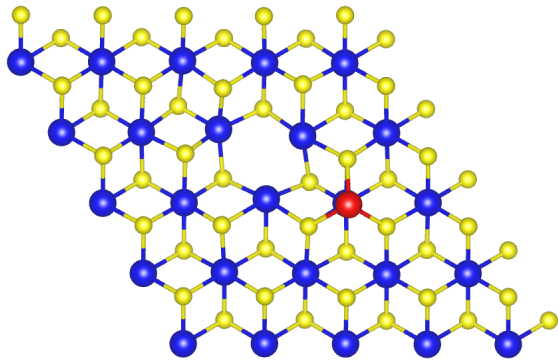
(f) Na at T_{Sn} site on pristine SnS_2



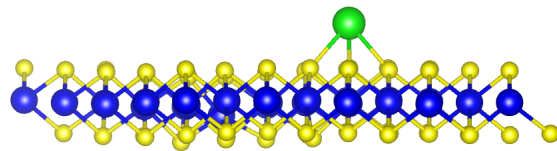
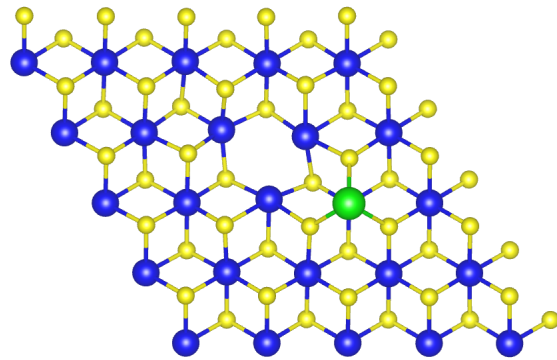
(g) Li at T_S site on pristine SnS_2



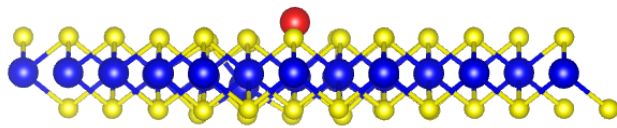
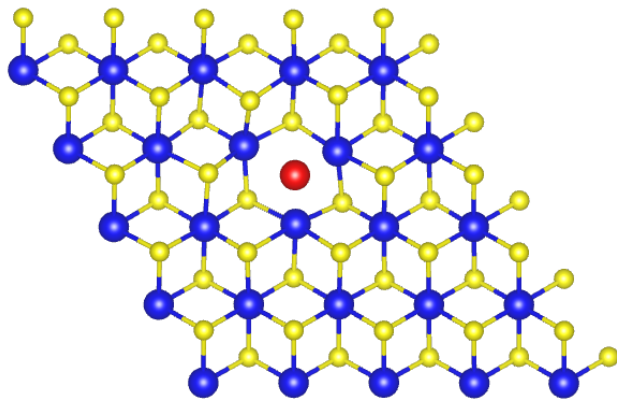
(h) Na at T_S site on pristine SnS_2



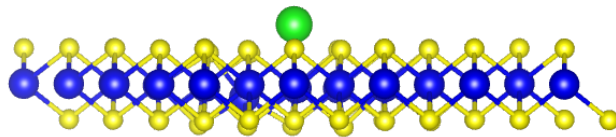
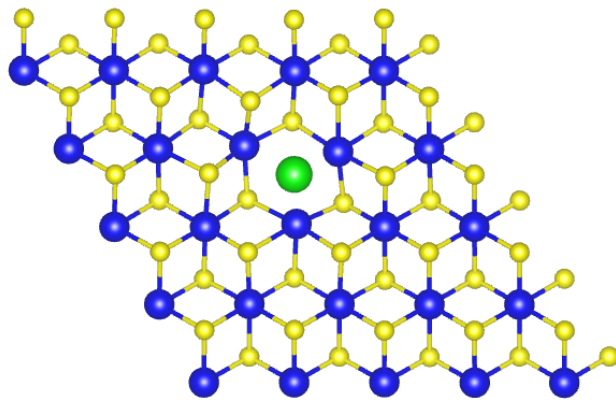
(i) Li at T_{Sn} site on S-vacancy SnS₂



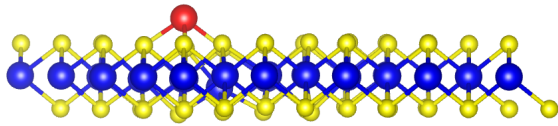
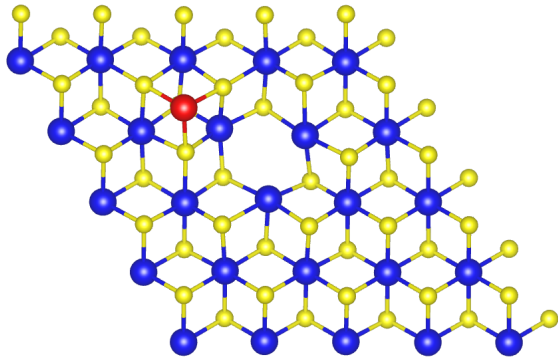
(j) Na at T_{Sn} site on S-vacancy SnS₂



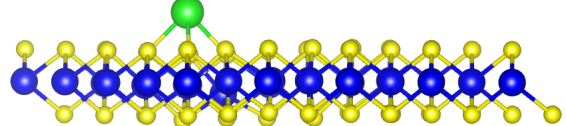
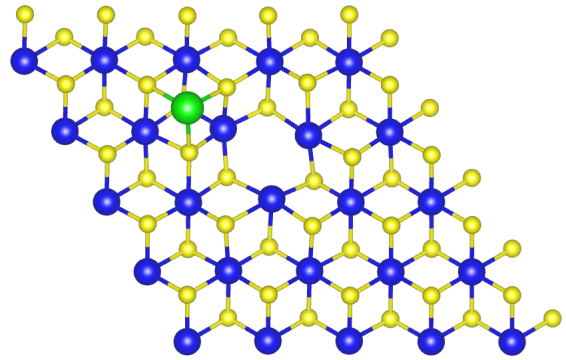
(k) Li at V_S site on S-vacancy SnS₂



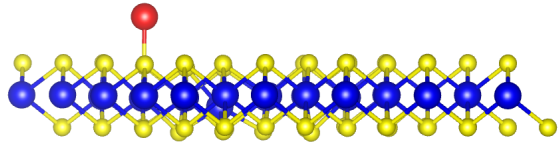
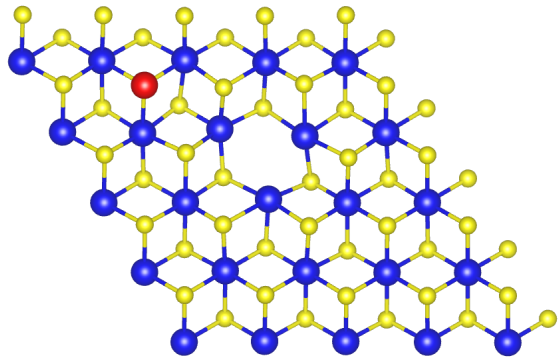
(l) Na at V_S site on S-vacancy SnS₂



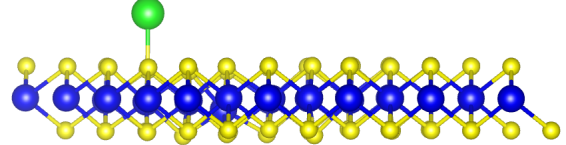
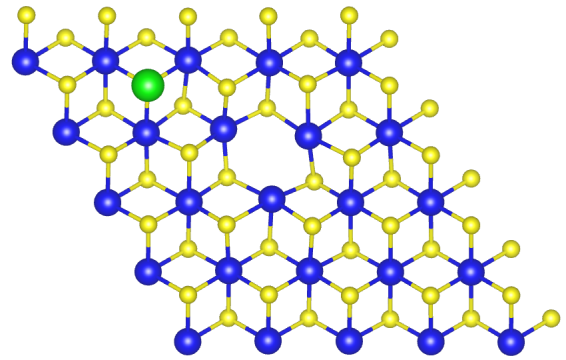
(m) Li at H_{SnS_2} site on S-vacancy SnS_2



(n) Na at H_{SnS_2} site on S-vacancy SnS_2

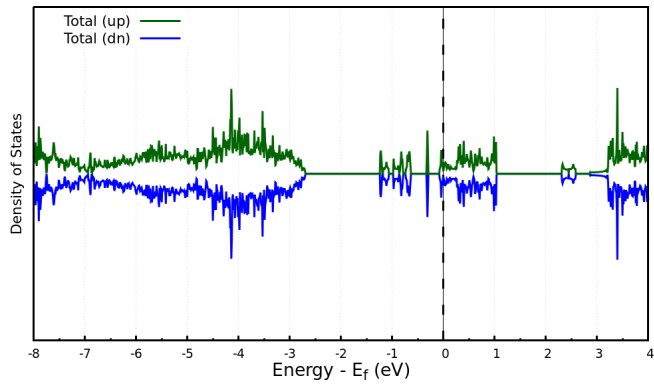


(o) Li at T_S site on S-vacancy SnS_2

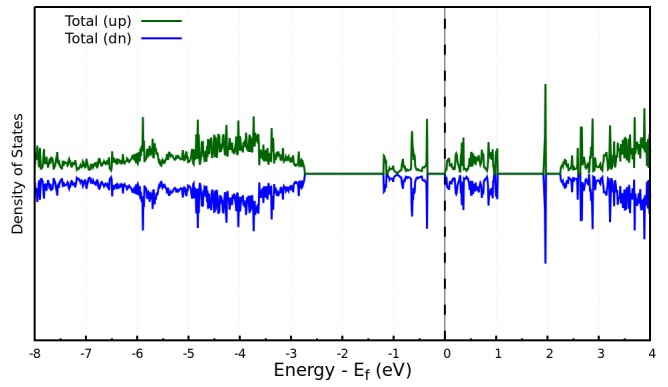


(p) Na at T_S site on S-vacancy SnS_2

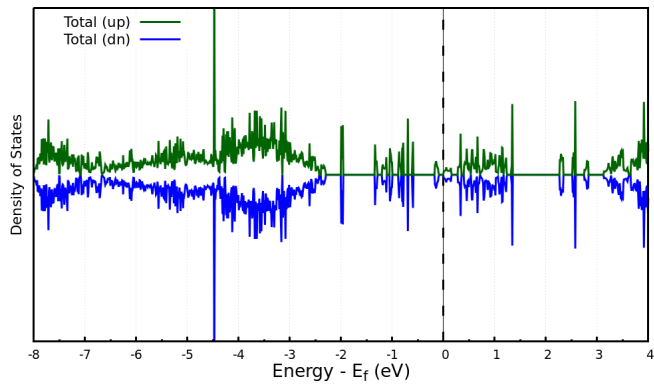
Figure 1: The relaxed various configurations (a-p) of Li/Na adatoms on the pristine and S-vacancy SnS_2 monolayer 5×5 supercell.



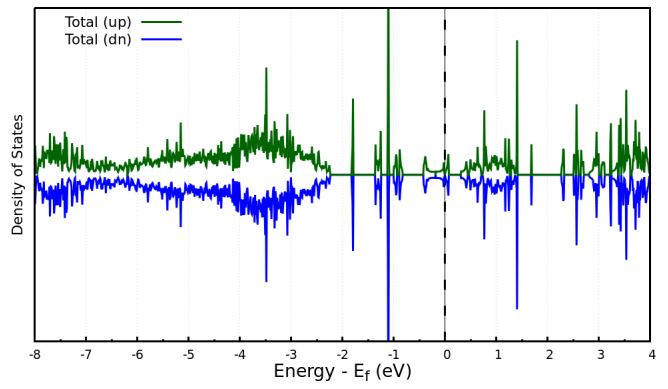
(a) 25 Li adatoms on pristine SnS_2



(b) 25 Na adatoms on pristine SnS_2



(c) 25 Li adatoms on SnS_2 with S-vacancy



(d) 25 Na adatoms on SnS_2 with S-vacancy

Figure 2 : The total density of states of multiple Li/Na adatoms on pristine SnS_2 monolayer as well as on SnS_2 monolayer with S-vacancy.