

Supporting Information

Adsorption and Diffusion of Lithium Polysulfides over Blue Phosphorene for Li-S batteries

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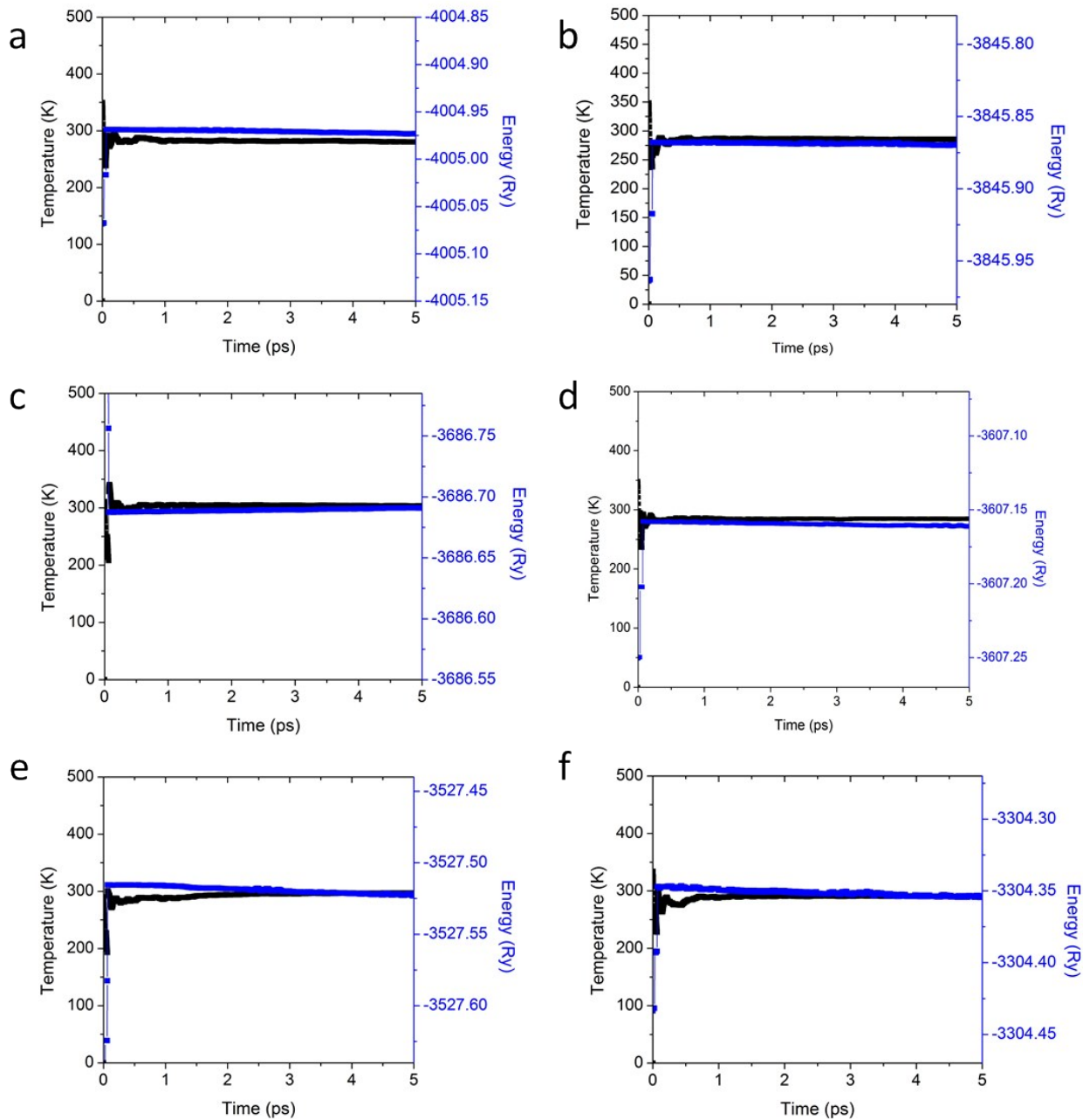


Figure S1: Time traces of temperature and total energy of a) Li_2S_8 b) Li_2S_6 c) Li_2S_4 d) Li_2S_3 e) Li_2S_2 and f) Li_2S over pristine BP obtained from AIMD simulations.

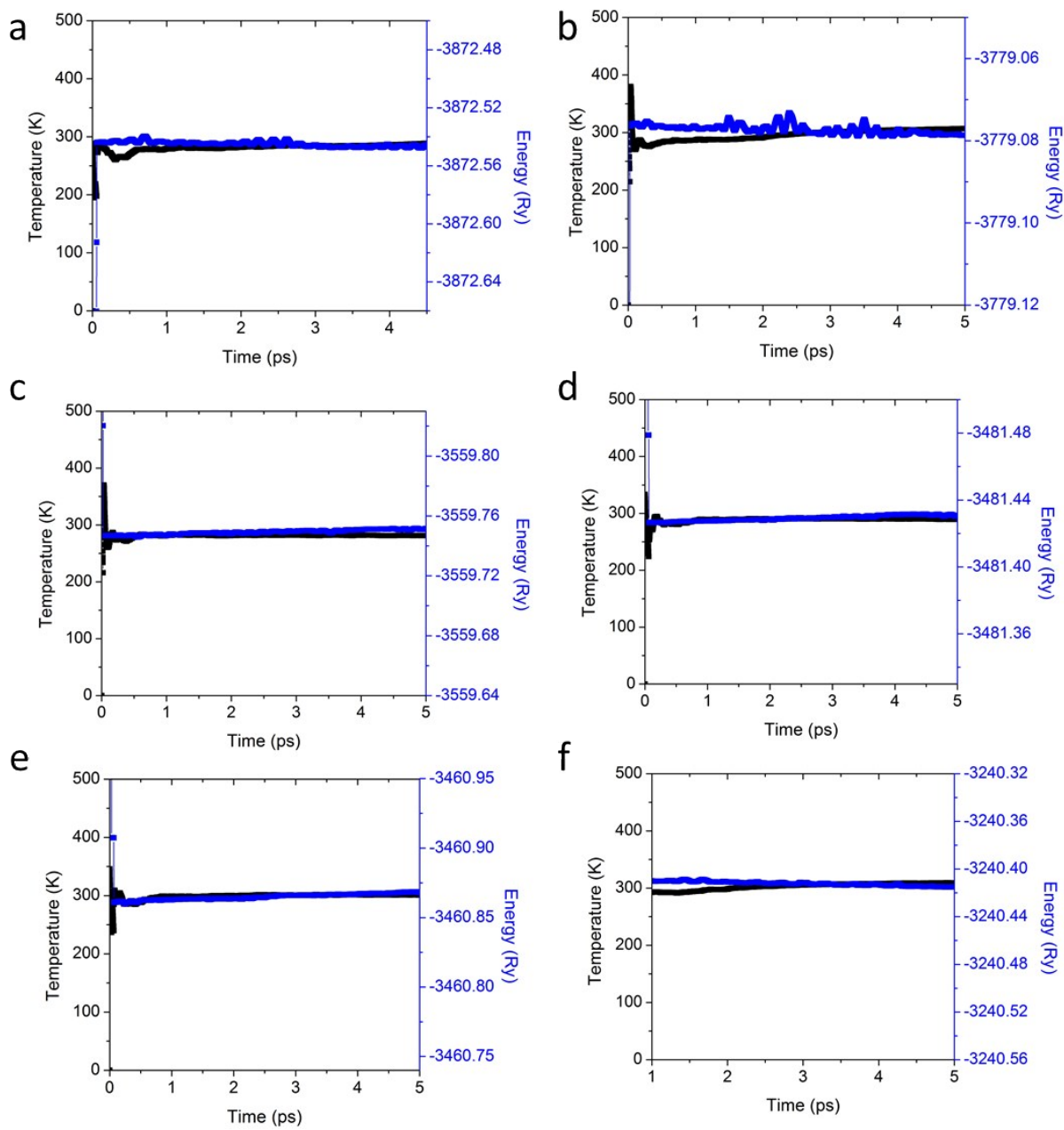


Figure S2: Time traces of temperature and total energy of a) Li_2S_8 b) Li_2S_6 c) Li_2S_4 d) Li_2S_3 e) Li_2S_2 and f) Li_2S over SVBP obtained from AIMD simulations.

Table S1: Legend for movie files showing the evolution of LiPSs on BP hosts at 300 K.

Movie #	Cathodic host	Description
1	Pristine BP	Li ₂ S
2		Li ₂ S ₂
3		Li ₂ S ₃
4		Li ₂ S ₄
5		Li ₂ S ₆
6		Li ₂ S ₈
7	Single vacancy BP	Li ₂ S
8		Li ₂ S ₂
9		Li ₂ S ₃
10		Li ₂ S ₄
11		Li ₂ S ₆
12		Li ₂ S ₈

Table S2: Comparison of energy barriers associated with the diffusion of Li, Na¹ and K¹ over pristine BP and their atomic radii.

Alkali metal	Diffusion barrier (ΔE)		Atomic radius (nm)
	Armchair	Zigzag	
Li	0.45	0.12	167
Na ^[1]	0.24	0.11	190
K ^[1]	0.11	0.093	243

Reference

1. Mukherjee, S.; Kavalsky, L.; Singh, C. V., Ultrahigh Storage and Fast Diffusion of Na and K in Blue Phosphorene Anodes. *ACS applied materials & interfaces* **2018**.