Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Superior Anchoring Effect of Cu-Benzenehexathial MOF as Aluminium-Sulfur Battery Cathode Host

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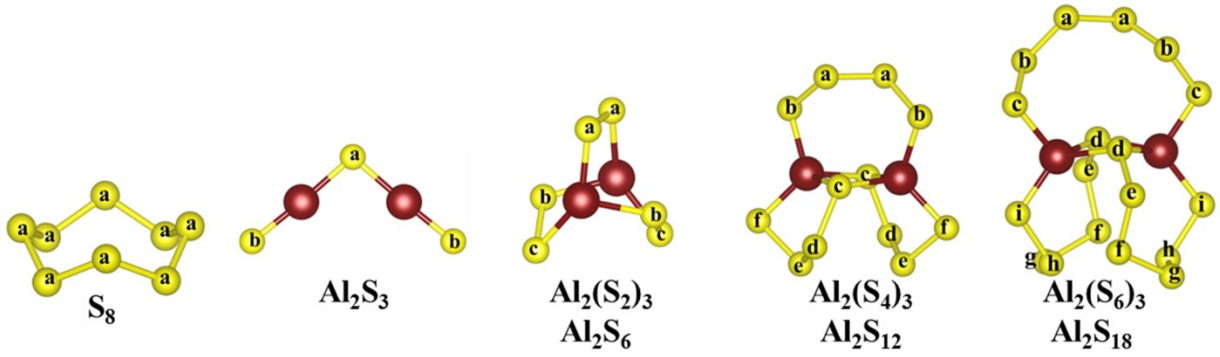

System	S-S (Å)									Al-S (Å)					
	a-a	a-b	b-c	c-d	d-e	e-f	f-g	g-h	h-i	Al-a	Al-b	Al-c	Al-d	Al-f	Al-i
S_8	2.06	-	-	-	-	-	-	-	-	-	-	-	-	-	
Al_2S_3	-	-	-	-	-	-	-	-	-	2.18	2.01	-	-	-	
Al_2S_6	2.12	-	2.14	-	-	-	-	-	-	2.24	2.33	2.18	-	-	
Al_2S_{12}	2.02	2.10	-	2.13	2.02	2.09	-	-	-	-	2.22	2.38	-	2.23	
Al_2S_{18}	2.06	2.08	2.07	-	2.11	2.01	2.10	2.03	2.07	-	-	2.24	2.35	-	2.23

Figure S1: Most stable molecular structures of S_8 and Al_2S_x (x = 3, 6, 12 and 18) representing non-equivalent sulfur atoms and their corresponding S-S and Al-S bond distances.

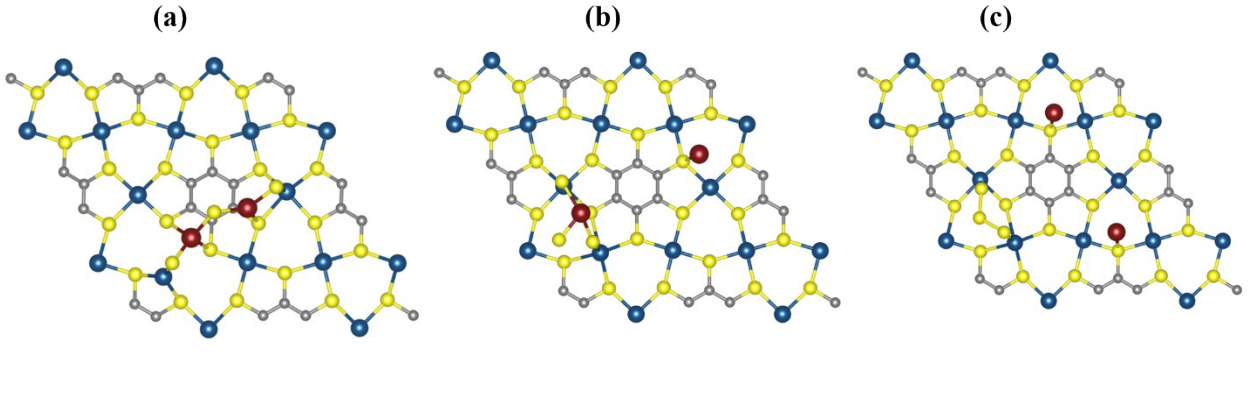

Figure S2: Top views of binding configurations (a) Al_2S_3, (b) $Al+AlS_3$ and (c) $Al+Al+S_3$ on Cu-BHT surface.

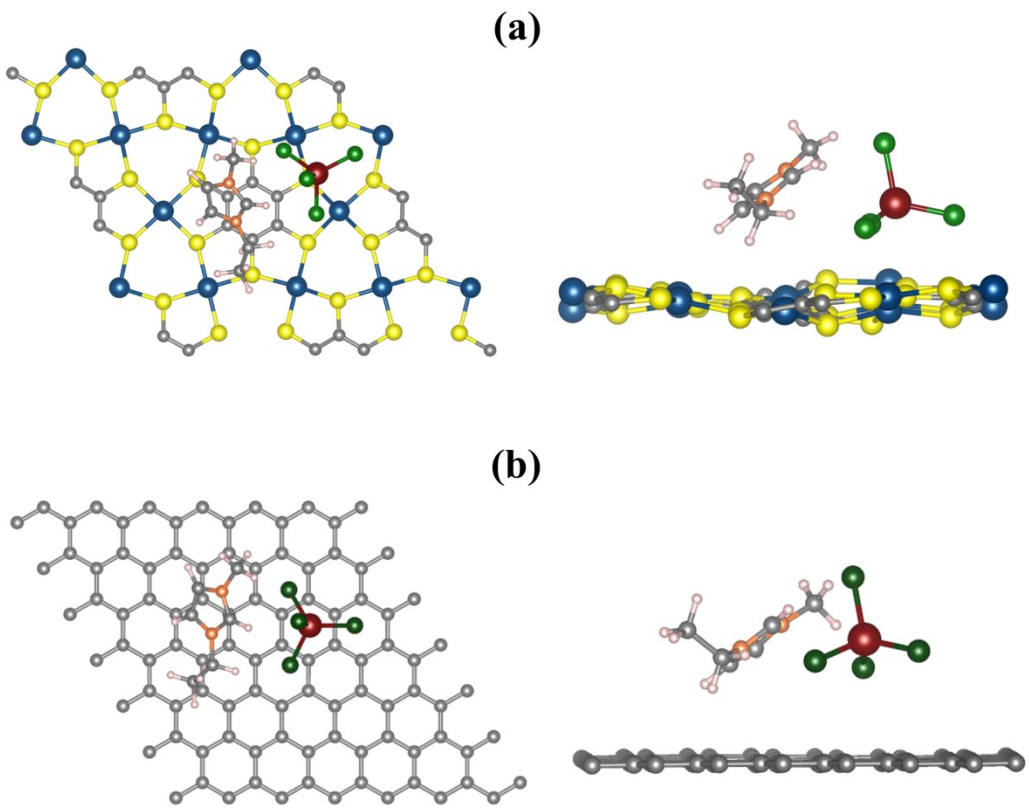

Figure S3: Top and side views of binding configurations of $EMIM^{+}AlCl_4^{-}$ electrolyte on (a) Cu-BHT monolayer, and (b) graphene surfaces.

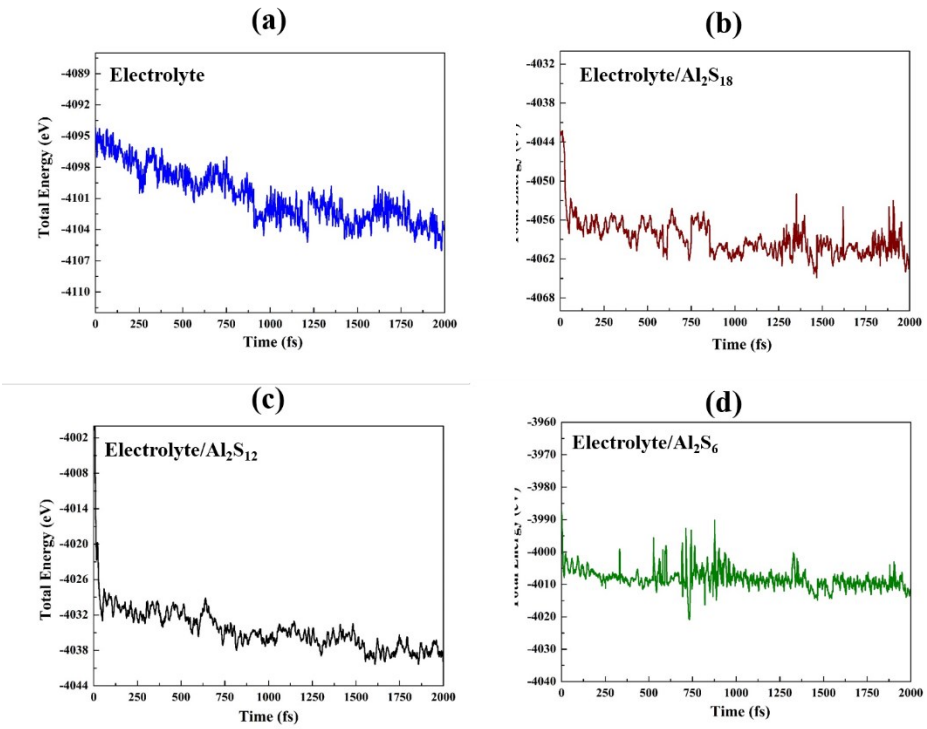

Figure S4: Total energy vs time plot of (a) $EMIM^{+}AlCl_4^{-}$ electrolyte, (b) $EMIM^{+}AlCl_4^{-}/Al_2S_{18}$, (c) $EMIM^{+}AlCl_4^{-}/Al_2S_{12}$, and (d) $EMIM^{+}AlCl_4^{-}/Al_2S_6$ for 2 ps AIMD simulations.

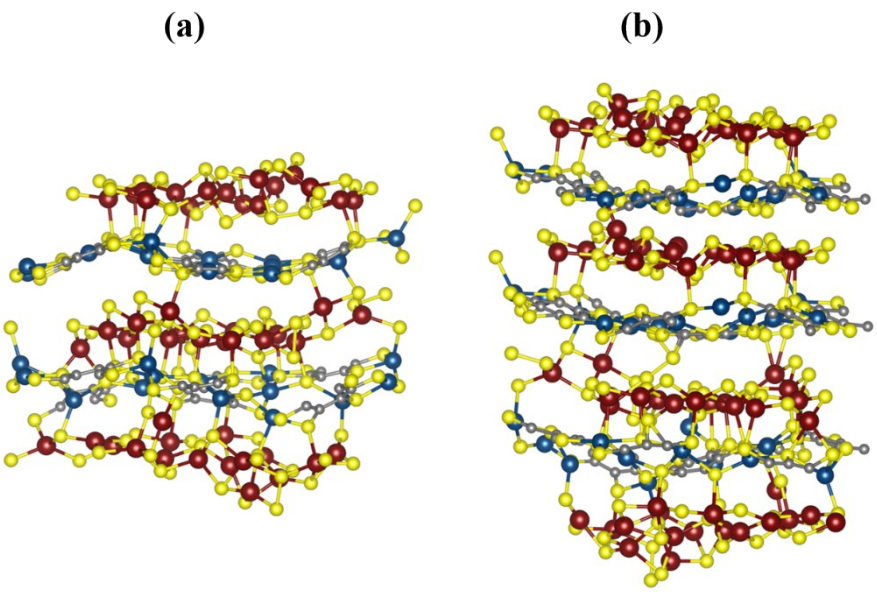

Figure S5: Side view of the optimized configuration with maximum stable loading of Al_2S_3 molecules on (a) Cu-BHT bilayer and (c) Cu-BHT trilayer surfaces. Here, for the clear understanding, the sulfur atoms of Al_2S_3 molecules and Cu-BHT monolayer surface are shown in orange and yellow colors, respectively.