Electronic Supporting Information (ESI)

Two-Dimensional $NiCl_2$ Monolayer as a Promising Multifunctional Anchoring Material in Sodium−Sulfur Batteries

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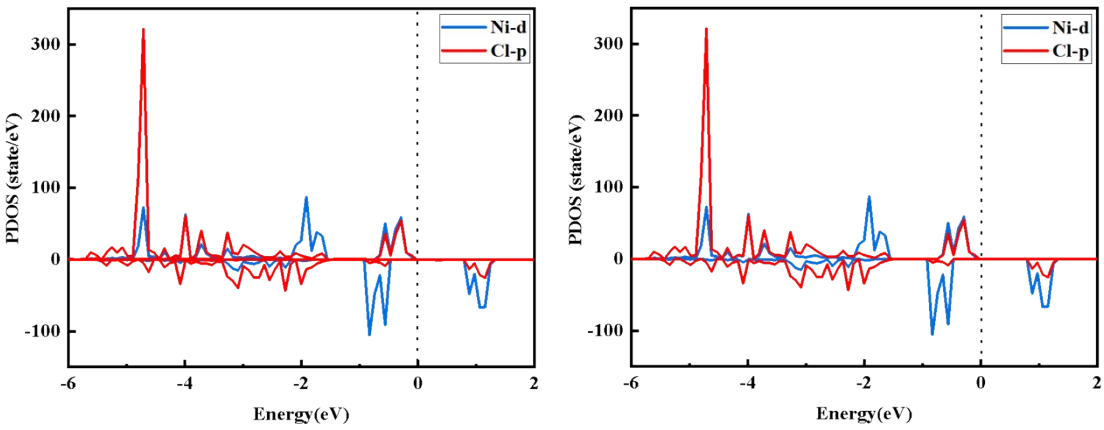
Table S1. The computed binding energies of S_8 and Na_2S_n intermediates on $NiCl_2$ monolayers using DFT+U and standard DFT methods.

	DFT+U	DFT
Na_2S	2.40	2.44
Na_2S_2	2.61	2.69
Na_2S_4	1.88	1.99
Na_2S_6	0.95	0.98
Na_2S_8	1.21	1.31
S_8	0.47	0.56

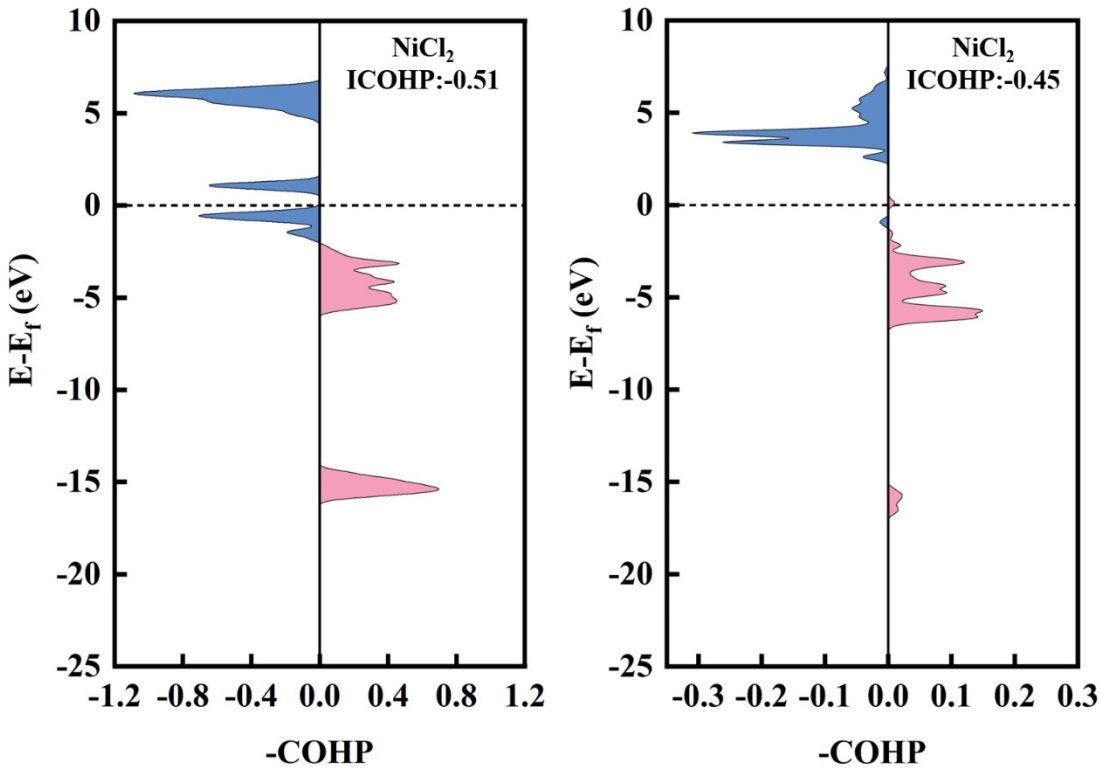
Table S2. The computed binding energies between long-chain Na_2S_n intermediates and DME/DOL

Na_2S_4/DME	0.59
Na_2S_6/DME	0.43
Na_2S_8/DME	1.07
Na_2S_4/DOL	0.65
Na_2S_6/DOL	0.84
Na_2S_8/DOL	0.93



(a) (b)

Fig. S1. The computed projected density of states (PDOSs) using (a) DFT+U and (b) DFT methods.



(a) (b)

Fig. S2. The computed crystal orbital Hamilton populations (COHPs), and integrated COHP (ICOHP) between Na atom of Na_2S_4 cluster and Cl atom of $NiCl_2$ using (a) DFT+U and (b) DFT methods.

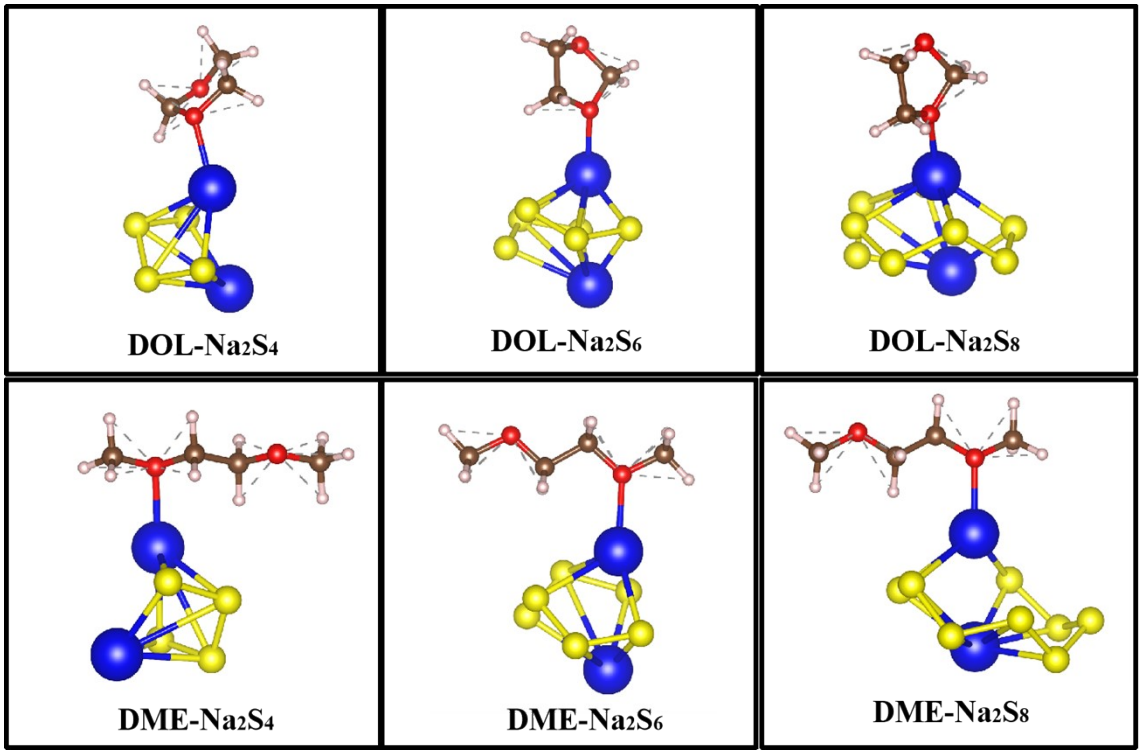


Fig. S3. The optimized structures for the interactions between Na_2S_n intermediates and DME/DOL.