

Effect of water molecules on the diffusions of alkali metal ions in two-dimensional transition metal sulfides

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Supporting Information

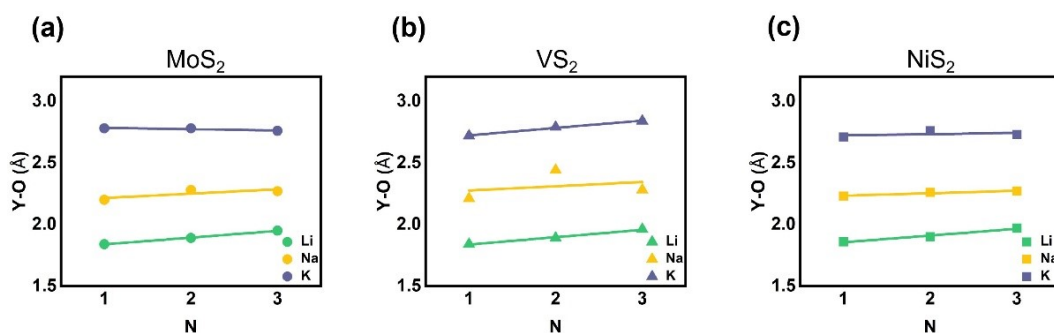


Figure S1. Evolution of Y-O bond lengths with hydration number in different 1T-phase metal sulfide systems. (a) 1T-MoS₂, (b) 1T-VS₂, and (c) 1T-NiS₂.

Table S1. Y-O bond lengths (Å) of hydrated alkali metal ion systems (Y·mH₂O) on 1T-MS₂ (M = Mo, V, Ni).

1T-MS ₂	Y	m		
		1	2	3
MoS ₂	Li	1.84	1.89	1.95
	Na	2.20	2.28	2.27
	K	2.78	2.78	2.76
VS ₂	Li	1.84	1.89	1.96
	Na	2.21	2.44	2.28
	K	2.72	2.79	2.84
NiS ₂	Li	1.86	1.90	1.97
	Na	2.23	2.26	2.27
	K	2.71	2.76	2.73

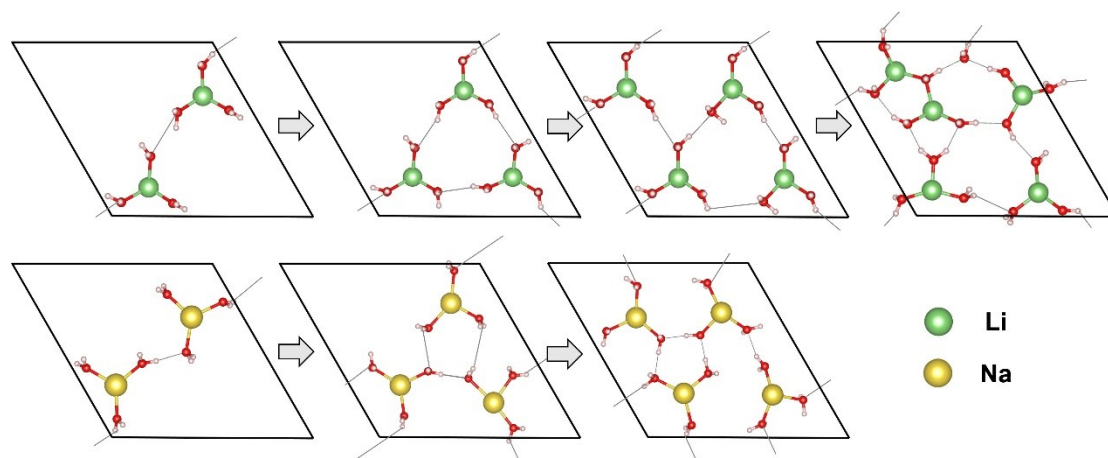


Figure S2. Evolution of hydrogen bond networks in different alkali metal hydrated ion systems. The green and yellow spheres represent Li and Na, respectively; the red and white spheres represent the oxygen and hydrogen atoms of water molecules, and the gray lines denote intermolecular hydrogen bonds.

Table S2. The variation in hydrogen bond lengths (\AA) of hydrated alkali metal ions $(Y \cdot 3H_2O)_n$ within MoS_2 layers.

Y	n					
	2	3	4	5	6	7
Li	2.33	2.33	2.25	1.95	1.80	1.66
Na	2.07	2.00	1.91	1.76	—	—

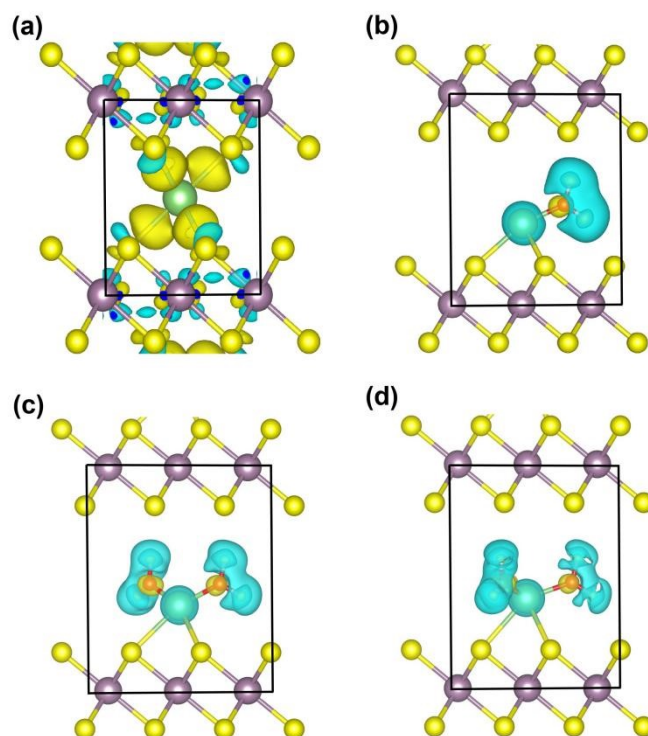


Figure S3. Differential charge density distributions of lithium ions with different degrees of hydration adsorbed on the 1T-phase MoS₂ surface. (a) Li adsorption system, (b) Li·1H₂O adsorption system, (c) Li·2H₂O adsorption system, (d) Li·3H₂O adsorption system. The yellow regions represent electron-rich zones, whilst the cyan regions represent electron-depleted zones; the purple, yellow and cyan spheres represent Mo, S and Li atoms respectively, the red and white spheres represent the O and H atoms in water molecules respectively.