Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for "A First-principles Investigation of ScO_2 Monolayer as Cathode Material for Alkali Metal-ion Batteries"

Zhixiao Liu,[1] Huiqiu Deng,[1, 2, *] Shiguo Zhang,[1, *] Wangyu Hu,[1] Fei Gao[1, 3]

[1]College of Materials Science and Engineering, Hunan University, Changsha 410082, China

[2]School of Physics and Electronics, Hunan University, Changsha 410082, China

[3]Department of Nuclear Engineering and Radiological Science, University of Michigan, Ann Arbor, MI 48109, USA

*Corresponding authors: hqdeng@hnu.edu.cn (H. Deng); zhangsg@hnu.edu.cn (S. Zhang)

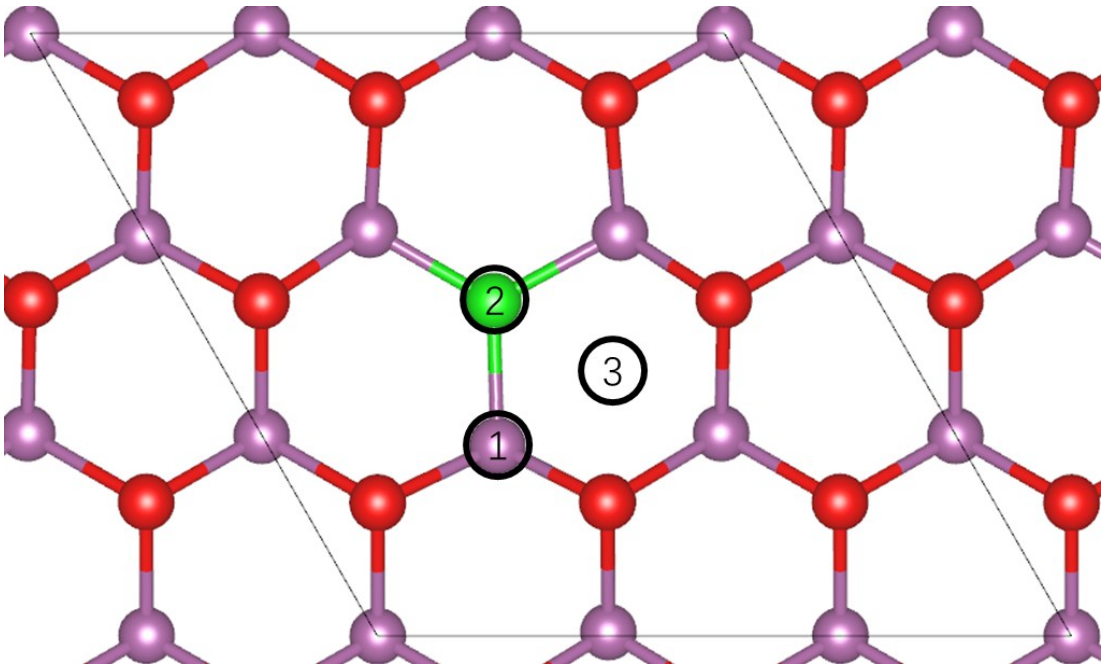

Figure S1. The O vacancy is generated by removing an O atom from the topmost atomic plane. The green sphere represents the O atom coordinating with the vacancy. Three typical sites are considered for investigating the effect of O vacancy on the alkali metal adsorption. The metal atom can be initially placed on (1) the first nearest atop-Sc site, (2) just above the vacancy which is named the atop-V site, and (3) the first nearest Hollow site.

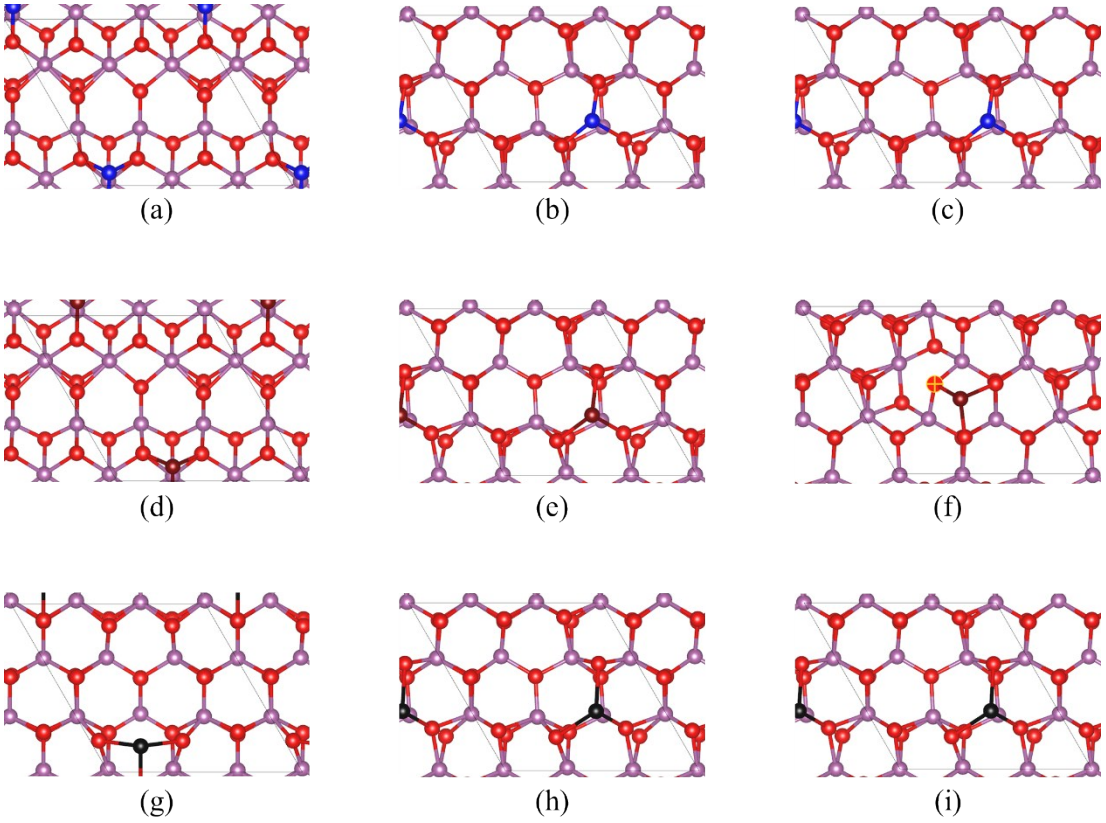

Figure S2. Optimized configurations of: (a)~(c) initially placing Li on the atop-Sc site, atop-V site and hollow site, respectively; (d)~(f) initially placing Na on the atop-Sc site, atop-V site and hollow site, respectively; and (g)~(i) initially placing K on the atop-Sc site, atop-V site and hollow site, respectively.

Table S1. Energetic and geometric properties of alkali metal atom adsorption on the H-ScO_2 (3×3) supercell with a vacancy.

Adsorbate	Initial	E^{ads}	D_{AM-Sc}	D_{AM-O}	Final

	Position	(eV)	(Å)	(Å)	Configuration
	atop-Sc	-9.38	2.53	2.00	Figure S2(a)
Li	atop-V	-3.92	3.09	2.10	Figure S2(b)
	hollow	-3.93	3.09	2.10	Figure S2(c)
	atop-Sc	-9.09	2.85	2.32	Figure S2(d)
Na	atop-V	-3.85	3.41	2.36	Figure S2(e)
	hollow	-4.77	3.20	2.28	Figure S2(f)
	atop-Sc	-3.41	3.51	2.71	Figure S2(g)
K	atop-V	-4.16	3.90	2.71	Figure S2(h)
	hollow	-4.16	3.90	2.71	Figure S2(i)