Supplementary materials

Stability and comparative analysis of two-dimensional AN_3 (A = Si, Sn) monolayers as host for K-ion storage: Insights from First-Principles calculations

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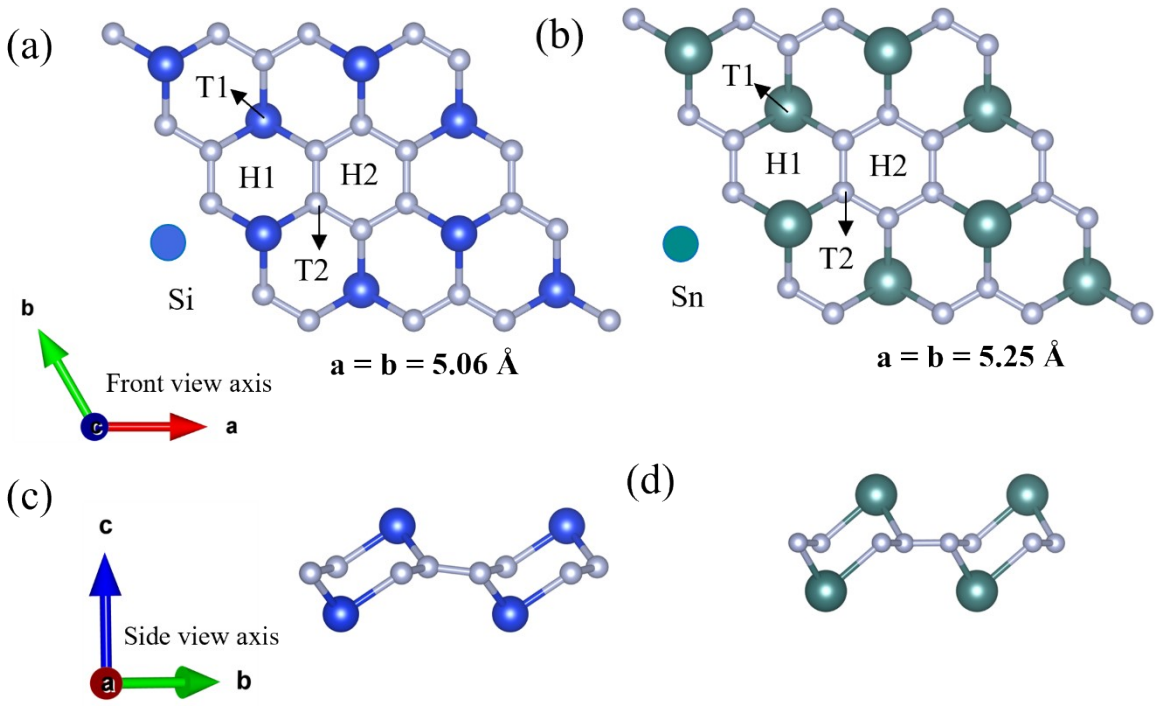

Fig. 1. Side and front view of the optimised SiN_3 and SnN_3 monolayers with selected sites for adsorption of K atom.

Table 1. the optimised 2 * 2 supercell structural lattice parameters of the XN_3 (X = Si, N) monolayers. The symbol a represents the lattice constant, the N-N and X-N bond are the distance between N with N atoms, and between X with N atoms.

2D-Structure	**a (Å)**	**N-N bond (Å)**	**X-N bond (Å)**
SiN_3	5.06 Å [This work] 5.06 Å [1] 5.08 Å [2]	1.36 Å 1.36 Å [1] 1.38 Å [2]	1.89 Å 1.89 Å [1] 1.88 Å [2]
SnN_3	5.25 Å [This work] 5.25 Å [3]	1.37 Å [3]	2.09 Å [3]

Table 2. Cohesive energy of the pristine SiN_3 and SnN_3 monolayers with other 2D monolayers materials.

Materials	**E_{coh} eV/atom**	**Ref.**
SiN_3	6.08 6.03	[1] [4]
SnN_3	6.87	This work
GeP_3	3.34	[5]
SnS	3.75	[6]
SnB	4.60	[7]
VC_4	5.2	[8]
SiP_3	5.01	[9]

Table 3. The phonon mode of the SiN_3 and SnN_3 monolayers, with other reported two-dimensional monolayers.

Structure	**Phonon frequency (cm^{-1})**	**Ref.**
SiN_3	1169	[1]
SnN_3	1386 1386	This work [3]
SiP_3	480	[9]
SbP_3	467	[10]
SnP_3	500	[11]
MoS_2	473	[12]
SnS	320	[6]
Si monolayer	580	[13]

The phonon band dispersion curve was calculated with the DFPT method using the Phonopy code [14]. The calculated phonon band spectrum of the SiN_3 and SnN_3 monolayers, shows no negative phonon mode of vibration in the entire Brillouin zone. These results verify the dynamic stability of the SiN_3 and SnN_3 monolayers and compare them with other 2D materials as illustrated in Table 3.

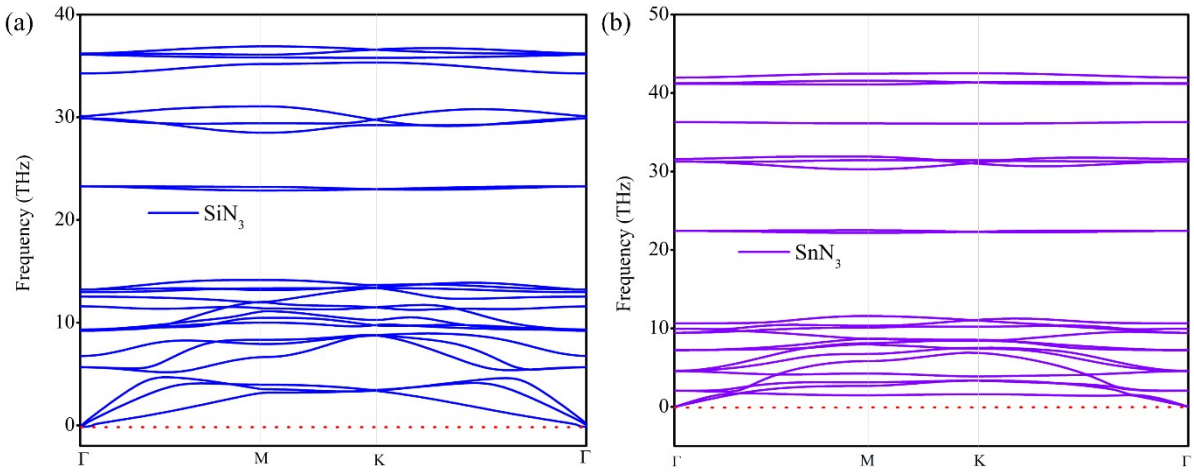

Fig. 2. Phonon band spectrum of the (a) SiN_3 and (b) SnN_3 monolayers.

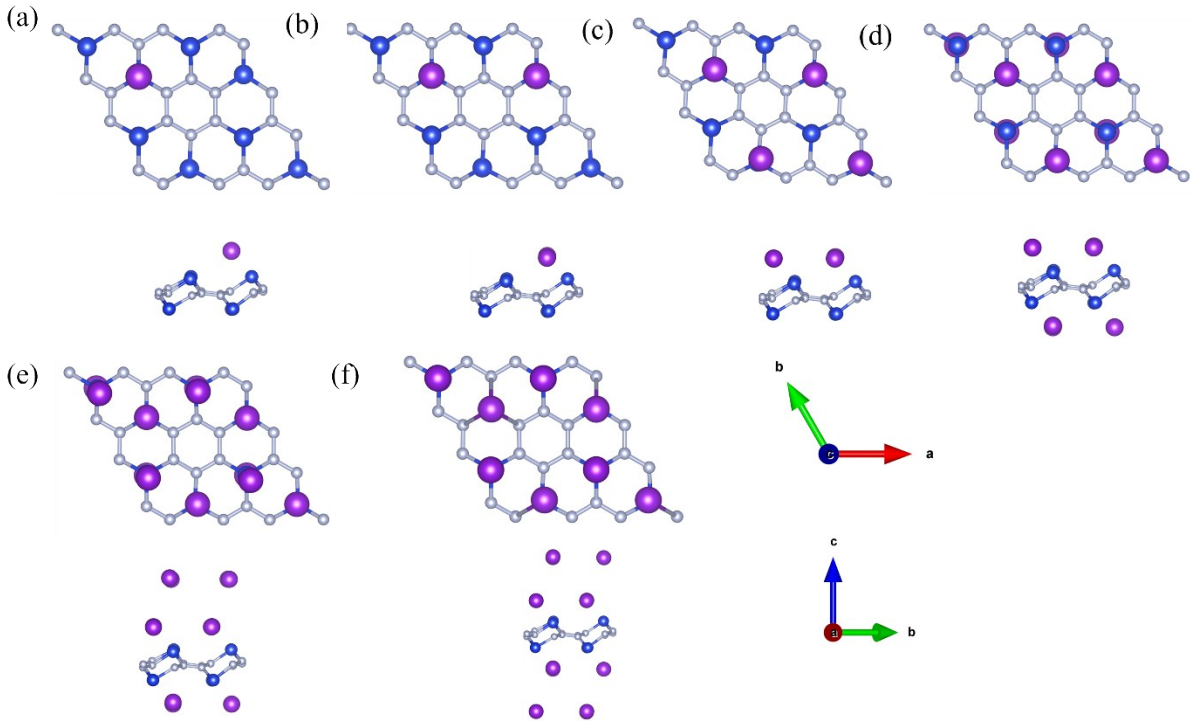

Fig. 3. Top and side views of various concentrations of potassium-ion over the SiN_3 monolayer in **(a-c)** single-sided and **(d-f)** double-sided configurations.

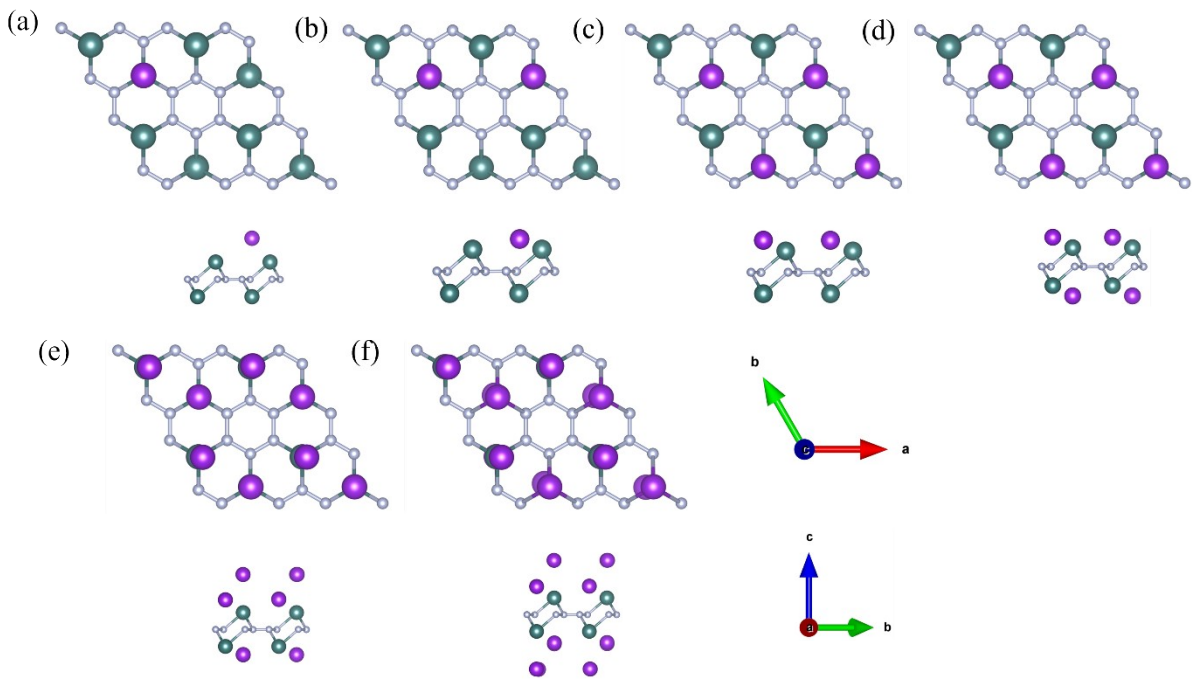

Fig. 4. Top and side views of various concentrations of potassium-ion over the SnN_3 monolayer in **(a-c)** single-sided and **(d-f)** double-sided configurations.

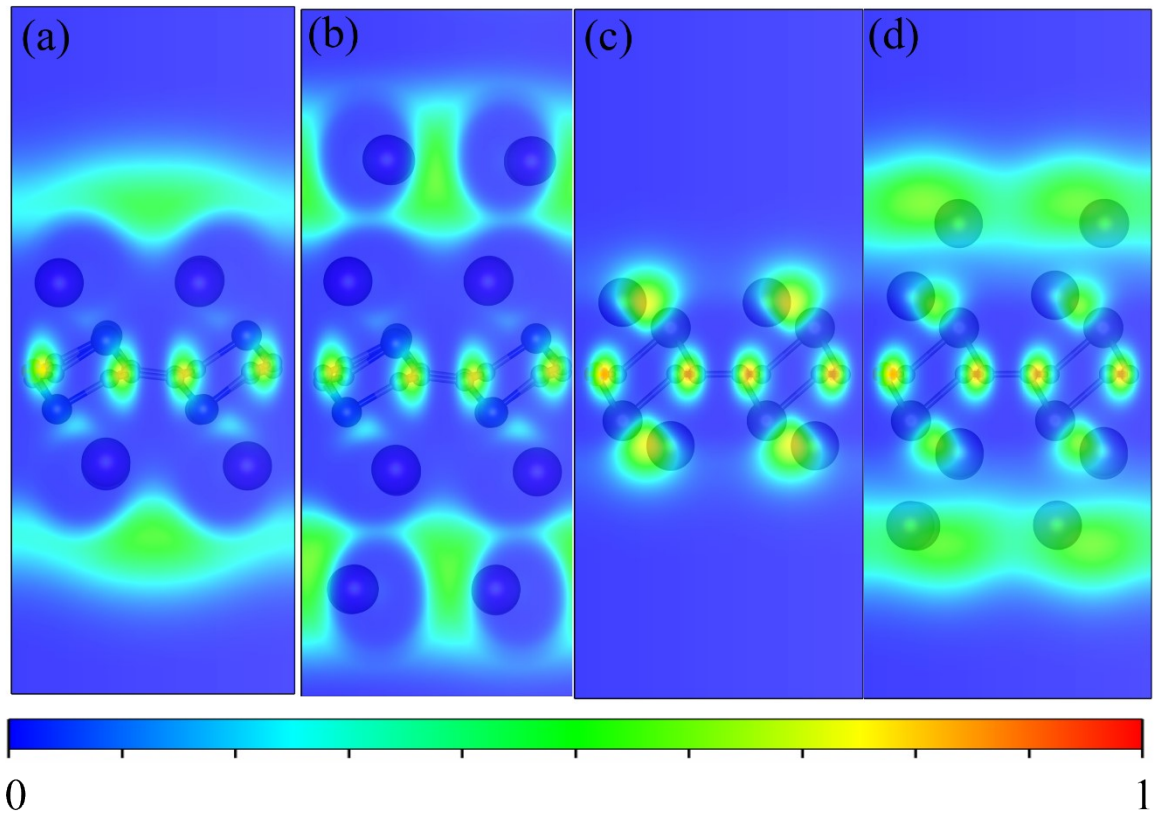

Fig. 5. Electron localisation function (ELF) map of (a) K_1SiN_3, (b) K_2SiN_3, (c) K_1SnN_3 and (d) K_2SnN_3.

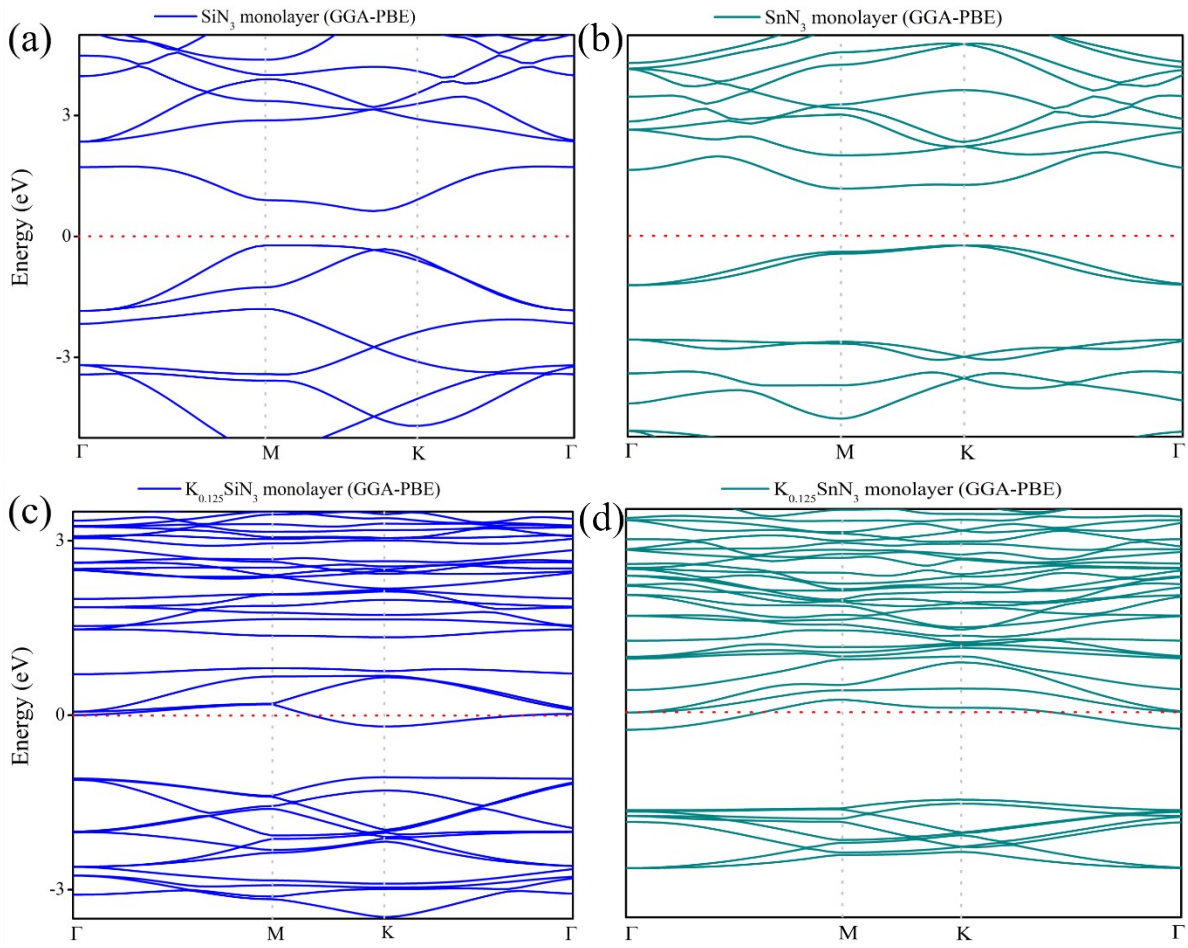

Fig. 6. Electronic band structure of the pristine (a) SiN_3 and (b) SnN3 monolayers, and K-adsorbed (c) $K_{0.125}SiN_3$ and (b) $K_{0.125}SnN_3$ monolayers, calculated using the GGA-PBE method.

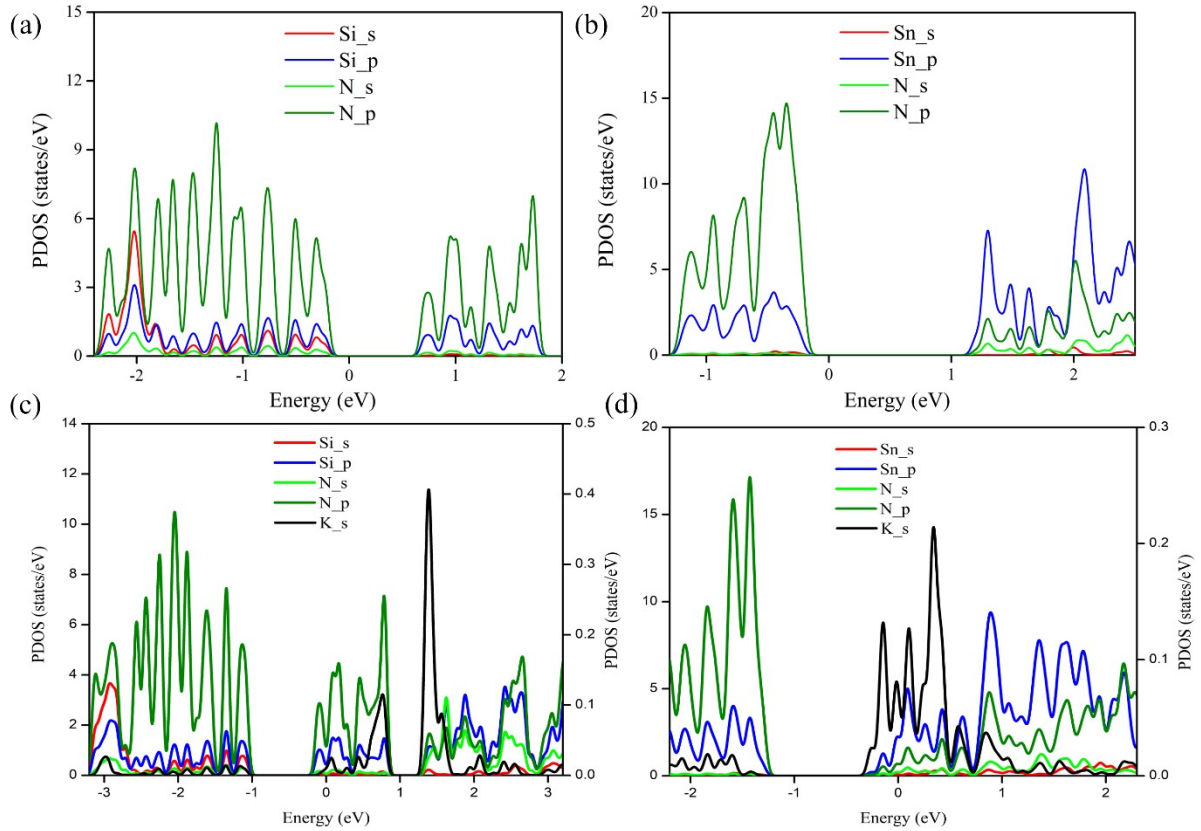

Fig. 7. Partial density of states (PDOS) of the pristine and $KSiN_3$ and $KSnN_3$ monolayers.

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