Supporting Information

Arsenene monolayer as an outstanding anode material for (Li/Na/Mg)-ion batteries: density functional theory

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1) Polymorph arsenene structural details:

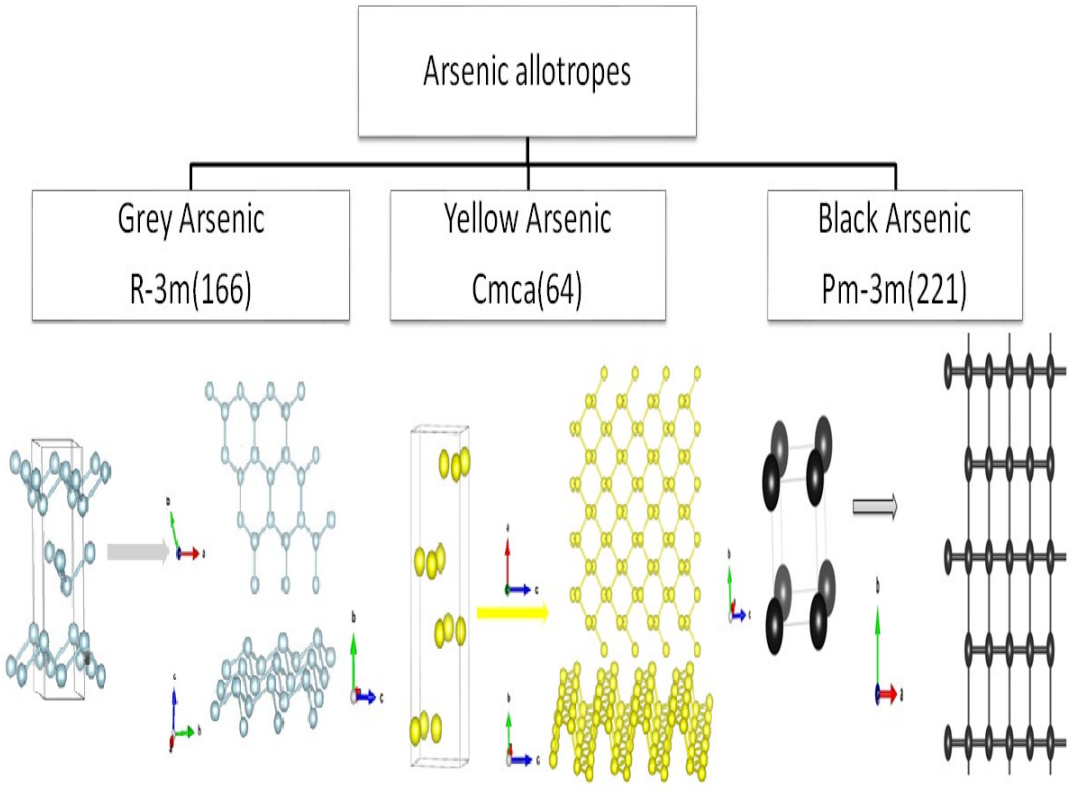


Figure S 1 : Three most common arsenic allotropes are metallic gray, yellow, and black arsenic, with gray being the most common and stable form

Table S 1: Calculated cohesive energies of arsenene buckling high, angles, As–As bond distances and bandgap obtained from GGA + vdW interaction included calculations.

	Latt. const. (Å)		Bond leng.	Bond ang.	Δ	E_c	Gap
	a	**b**	(Å)	(deg)	(Å)	(eV)	(eV)
Buckled	3,83	3,83	2,60	94,57	1,43	-2,95	1,99 (Indirect)
Puckred	4,00	4,48	2,62-2,68	97,584	2,62	-2,89	0,91(Indirect)
Planar	5,43	5,43	2,71	90	0	-2,32	0,19

After the energy minimization and geometry optimization, the obtained lattice parameters, band length, Δ and gap are shown in Table S1.

In order to explore the stability of each structure the cohesive energy, E_c, was investigated. As it can be observed, two types of structures, buckled and puckered, are found to be stable.

2) Adsorption of single adatoms on arsenene

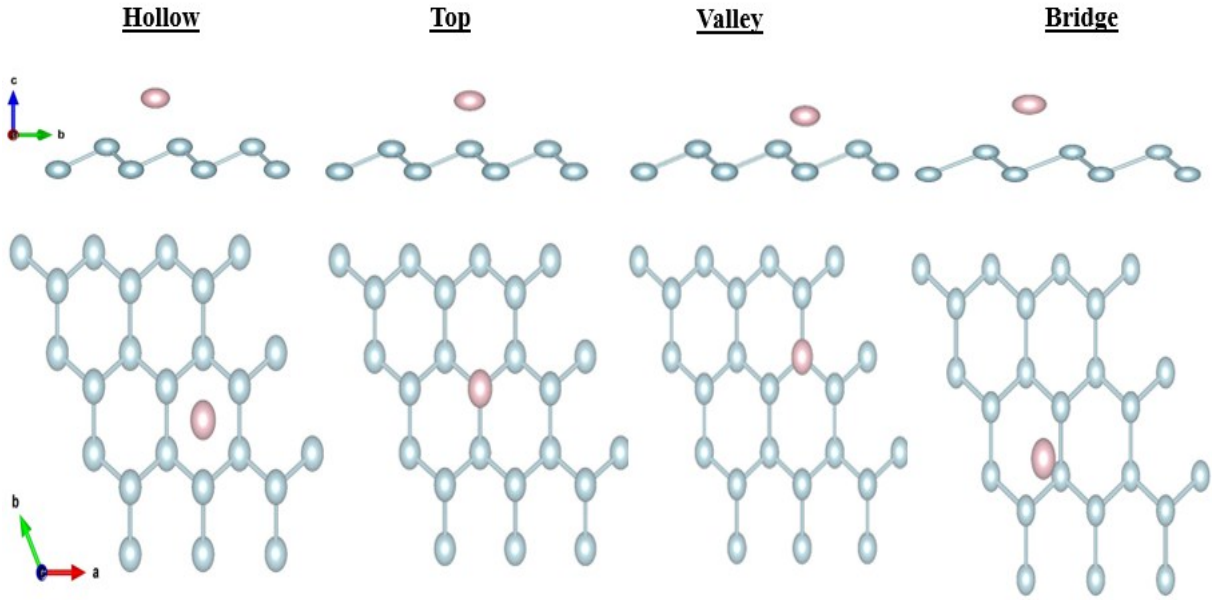


Figure S 2: Structure of arsenene nanosheet and the schematics of the possible adatoms absorption sites in top and side views.

Table S 2: Adsorption energies at different adsorption sites, vertical distance (h) at the V-site

Adatoms	E_{ad}(eV)				h(Å)
	Arsenene				
	H	T	V	B	
Li	-2,413	-2,169	-2,554	Move to V	1,37
Na	-1,852	-1,472	-1,913	-1,827	2,169
Mg	-0,735	-0,646	-1,107	-0,717	2,0117

Figure S1 : (a) Top and (b) side views of atomic configuration in LiAs lattice. with bond lengths and thickness

3) Lattice parameters and interatomic distances for Li_xAs, Na_xAs and Mg_xAs

	Lattice parameters (Å)		bond lengths (Å)		Lattice parameter change (%)
	a	b	As-As	M-As	
Li_xAs					
$Li_{0,125}As$	3,87	3,87	2,65	2,68	1,04
$Li_{0,375}As$	4,02	3,99	2,73	2,66	4,96
$Li_{0,5}As$	4,05	3,97	2,83	2,68	5,74
LiAs	4,06	4,06	2,74	2,66	6,01
Li_2As	4,11	4,11	2,57	2,59	7,31
Li_3As	4,20	4,20	2,62	2,54	9,66
Na_xAs					
$Na_{0,125}As$	3,89	3,36	2,60	3,11	1,54
$Na_{0,25}As$	3,91	3,89	2,63	3,13	2,05
$Na_{0,375}As$	3,90	3,89	2,61	3,14	1,79
$Na_{0,5}As$	3,91	3,90	2,63	3,16	2,05
$Na_{0,625}As$	3,90	3,89	2,63	3,14	1,79
$Na_{0,75}As$	3,90	3,87	2,63	3,15	1,79
$Na_{0,875}As$	3,89	3,87	2,73	3,18	1,54
NaAs	3,88	3,86	2,70	3,17	1,29
$Na_{1,5}As$	3,79	3,27	2,64	3,21	-1,06
Na_2As	3,76	3,34	2,62	3,22	-1,86
Na_3As	3,81	3,83	3,15	2,87	-0,52
Mg_xAs					

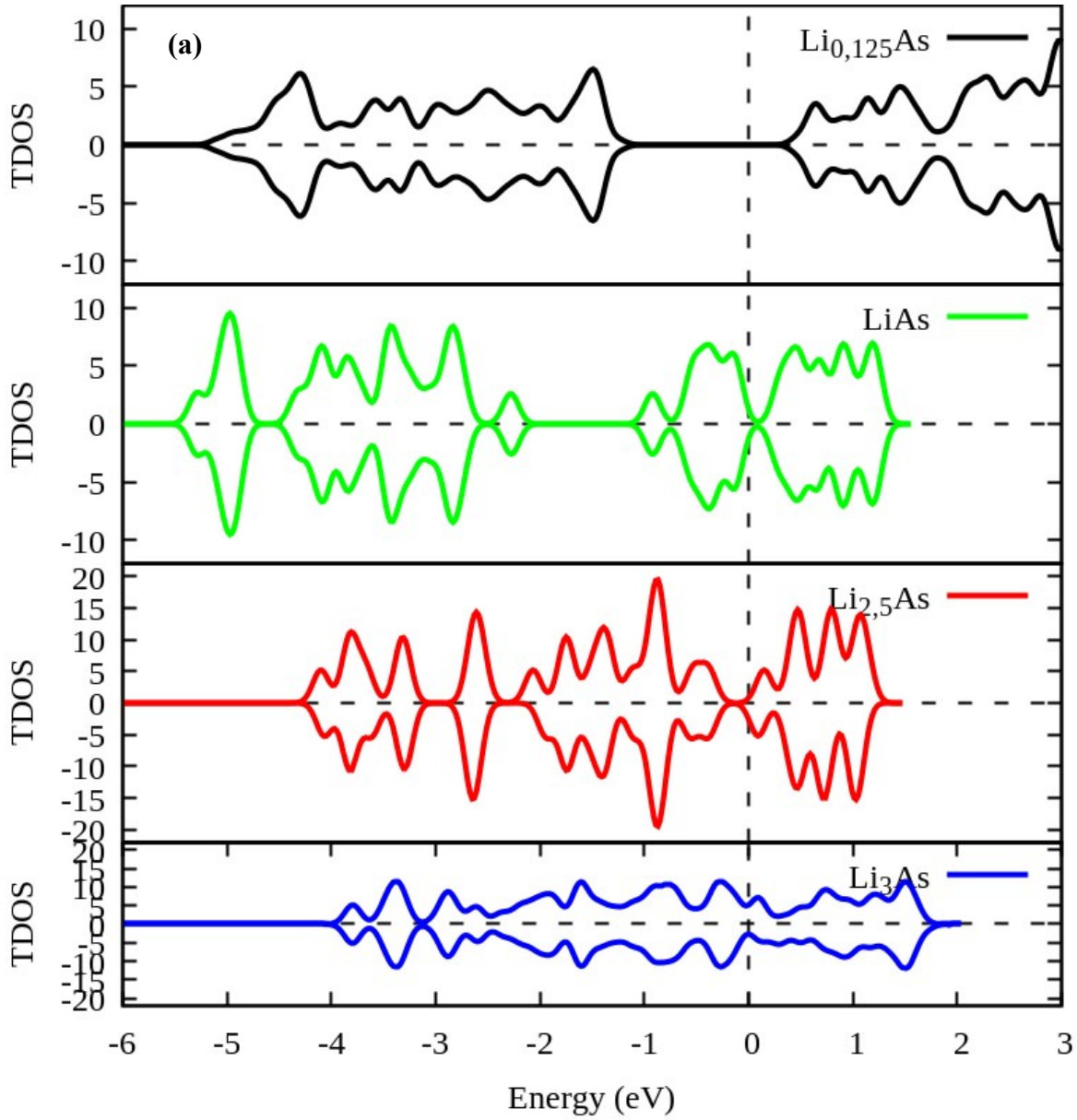
$Mg_{0,125}As$	3,84	3,84	2,58	3,09	0,26
$Mg_{0,25}As$	3,71	3,71	2,59	3,29	-3,23
$Mg_{0,375}As$	3,61	3,61	2,57	3,41	-6,09
$Mg_{0,5}As$	3,52	3,52	2,57	3,55	-8,81
MgAs	3,40	3,40	2,49	3,58	-12,65
Mg_2As	3,83	3,83	2,62	3,76	0,00

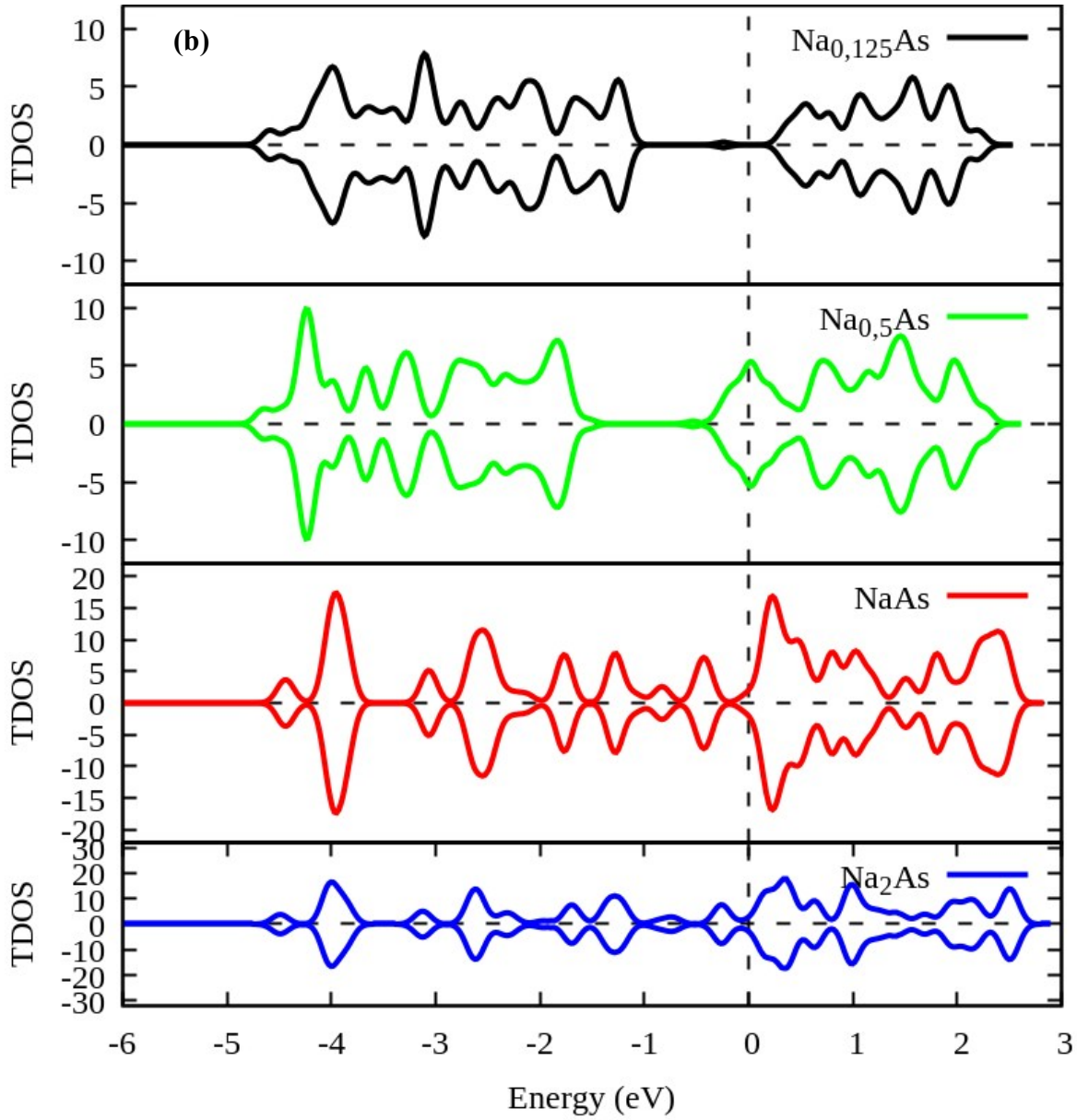
Table S 3 : Calculated lattice parameters, interatomic bonds and lattice parameters change

4) Magnetism behavior

Table S 4: The calculated results for the partial and total magnetic moments per unit cell

M_xAs	Magnetic moment		
	As (μ_B/atom)	Ad-atoms (μ_B/atom)	Total (μ_B/cell)
$Li_{0,125}As$	-0,0001	0,0001	0,00
LiAs	0,0011	-0,0018	-0,02
$Li_{2,5}As$	0,0038	-0,0034	0,00
Li_3As	0,0005	0,0058	0,027
$Na_{0,125}As$	-0,0002	-0,0001	0,00
$Na_{0,5}As$	-0,0002	-0,0001	0,00
NaAs	-0,0000	0,0000	0,00
Na_2As	-0,0001	0,0000	0,00
$Mg_{0,125}As$	-0,0002	-0,0026	0,00
$Mg_{0,5}As$	0,0000	0,0000	0,00
MgAs	0,0054	0,0078	0,03
Mg_2As	-0,0075	-0,0239	-0,08


(a)
Li0,125As
LiAs
Li2,5As
Li3As
TDOS
TDOS
TDOS
TDOS
Energy (eV)


(b)
Na0,125As
Na0,5As
NaAs
Na2As
TDOS
Energy (eV)

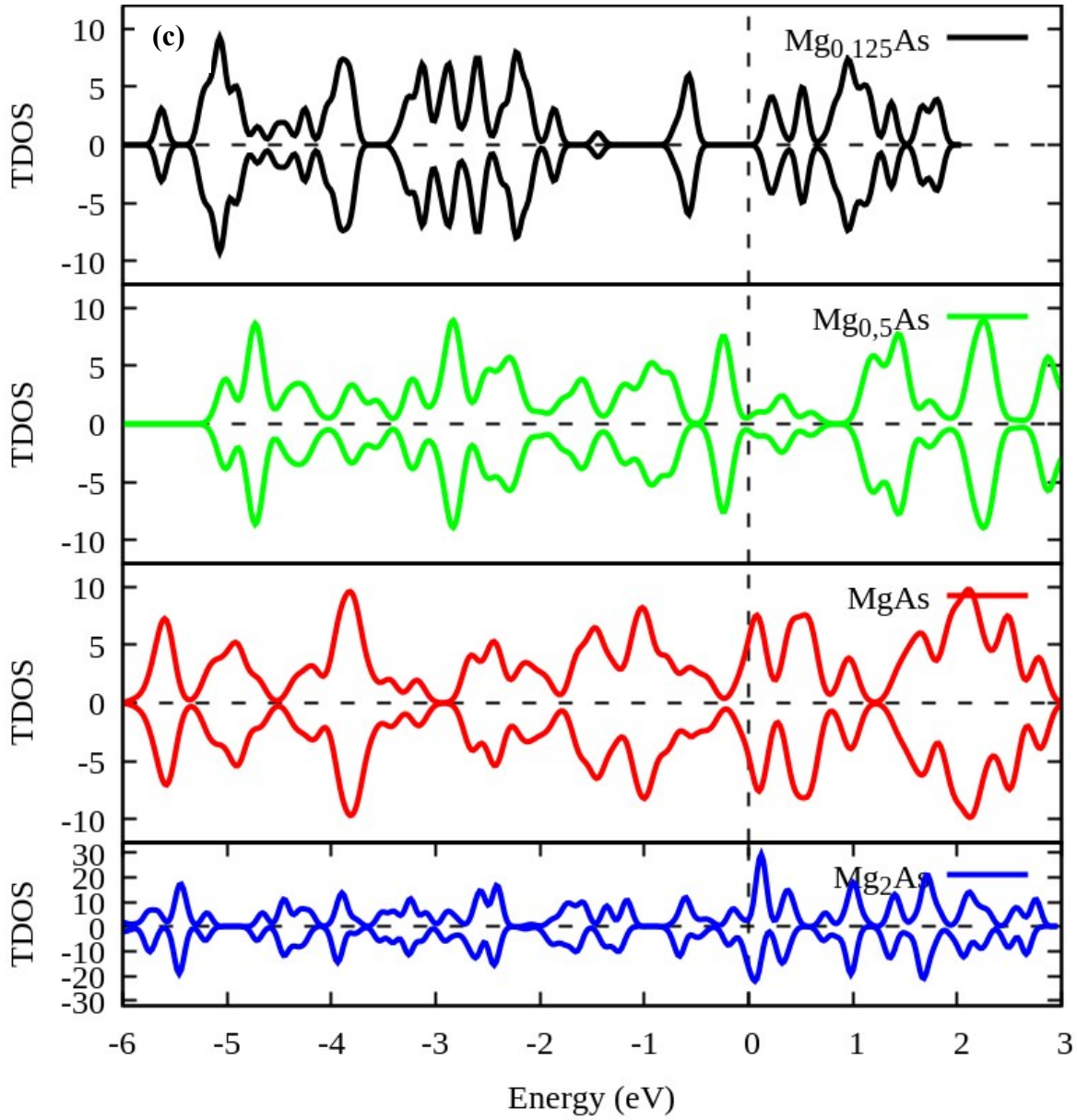


Figure S 3: Total density of states (DOS) of Li_xAs, Na_xAs ,and Mg_xAs. (The Fermi level is aligned to 0.)