Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary data to

Tunable electronic properties and band alignments of InS-arsenene heterostructure via external strain and electric field

Hui Yao,[a,b] Chao Zhang,[c] Qiang Wang,[a] Jianwei Li,[a] YunjinYu,[a] Fuming Xu,[†a] Bin Wang[*a] and Yadong Wei [a]

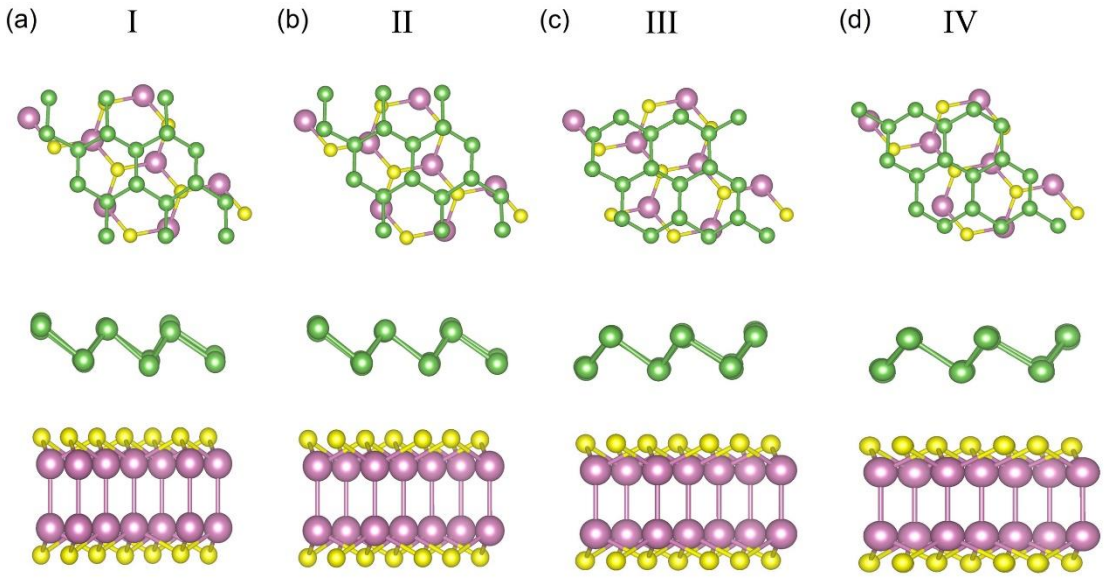
[a] *Shenzhen Key Laboratory of Advanced Thin Films and Applications, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, 518060, China.*
[b] *Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen, 518060, China.*

[c] *Beijing Computational Science Research Center, Beijing, 100193, China.*

E-mail address: binwang@szu.edu.cn; xufuming@szu.edu.cn.

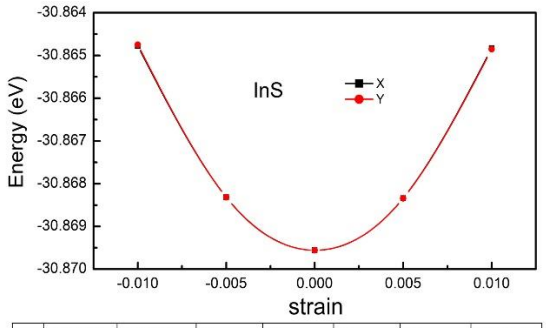
Supplementary Figures

Figure S1.(color online) Top and side views of InS-Aresenene vdWH with different stacking patterns. (a) The first As atom of upper aresenene layer align with S atom, (b) (a) The first As atom of upper aresenene layer align with In atom, (c) The first As atom of lower aresenene layer align with S atom, (d) The first As atom of lower aresenene layer align with In atom. The I stacking pattern has the lowest binding energy.

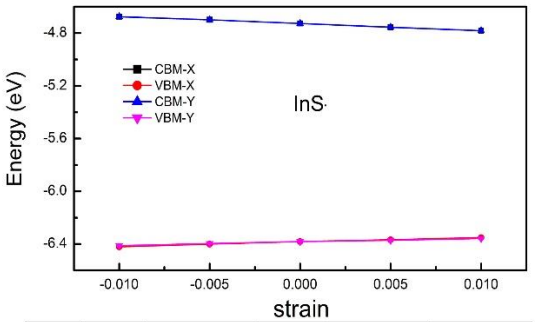


Stacking patterns	I	II	III	IV
Binding Energy (meV/Å)	-113.2	-112.4	-111.9	111.3

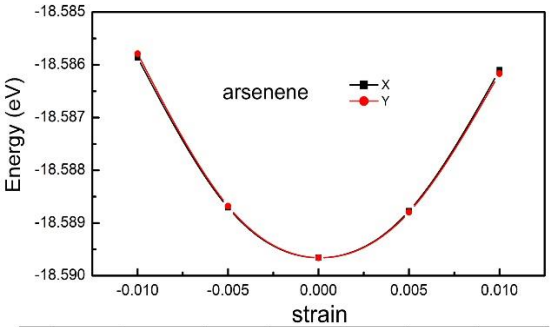
Figure S2.(color online) The left column : elastic modulus C_{2D}, and right column: deformation potential constant E_{DP} at different directions for isolated InS monolayer, arsenene monolayer and InS-arsenene vdWH.



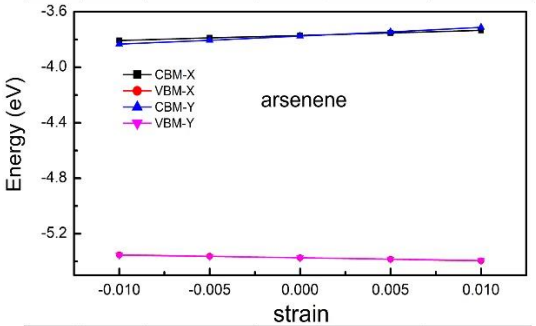
	Intercept Value	Intercept Standard Error	B1 Value	B1 Standard Error	B2 Value	B2 Standard Error	Statistics Adj. R-Square
X	-30.86953	1.98119E-5	-0.00246	0.0018	47.29866	0.3039	0.99983
Y	-30.86953	2.0920E-5	-0.00466	0.0019	47.32271	0.3209	0.99982



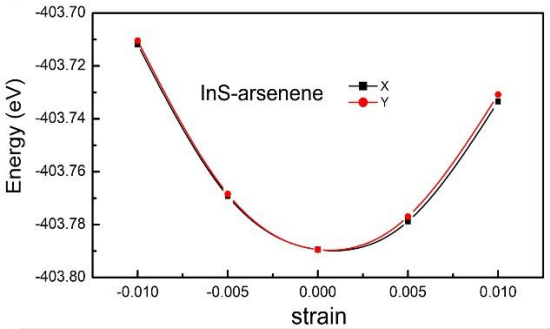
	Intercept Value	Intercept Standard Error	Slope Value	Slope Standard Error	Statistics Adj. R-Square
CBM-X	-4.7278	7.0007E-4	-5.3483	0.0990	0.9886
VBM-X	-6.3846	1.0900E-4	3.4695	0.0154	0.9991
CBM-Y	-4.7277	7.0524E-4	-5.3847	0.0997	0.9880
VBM-Y	-6.3843	9.6594E-4	2.6817	0.0136	0.9997



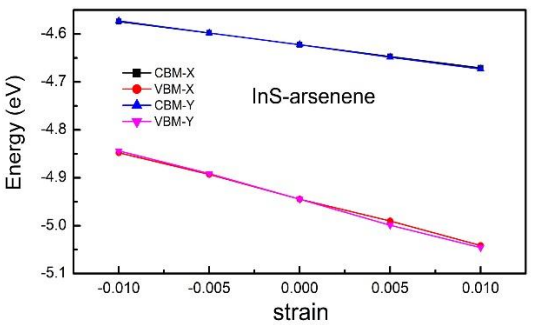
	Intercept Value	Intercept Standard Error	B1 Value	B1 Standard Error	B2 Value	B2 Standard Error	Statistics Adj. R-Square
X	-18.58966	1.7007E-5	-0.01064	0.00154	36.75951	0.26088	0.99980
Y	-18.58966	2.2541E-5	-0.01726	0.00205	36.80714	0.34577	0.99965



	Intercept Value	Intercept Standard Error	Slope Value	Slope Standard Error	Statistics Adj. R-Square
CBM-X	-3.7708	1.3727E-4	3.6467	0.0194	0.9998
VBM-X	-5.3739	2.2717E-4	-2.3515	0.0321	0.9991
CBM-Y	-3.7744	7.9586E-4	6.2622	0.1125	0.9986
VBM-Y	-5.3740	2.8803E-4	-2.3165	0.0407	0.9982



	Intercept Value	Intercept Standard Error	B1 Value	B1 Standard Error	B2 Value	B2 Standard Error	Statistics Adj. R-Square
X	-403.7902	6.6788E-4	-1.05200	0.06061	674.6150	10.2449	0.99914
Y	-403.7897	5.1969E-4	-0.98454	0.05100	690.4335	8.62020	0.99941



	Intercept Value	Intercept Standard Error	Slope Value	Slope Standard Error	Statistics Adj. R-Square
CBM-X	-4.6225	1.0693E-4	-4.8438	0.0151	0.9999
VBM-X	-4.9454	1.6900E-4	-7.6928	0.0239	0.9988
CBM-Y	-4.6229	1.4942E-4	-5.0192	0.0211	0.9999
VBM-Y	-4.9449	1.7780E-4	-8.0414	0.0260	0.9968

Figure S3.(color online) The band structures of (a) InS monolayer, (b) aresenene(As) monolayer and (c) InS-As vdWH at HSE level. In each panel, the Fermi level is set to zero.

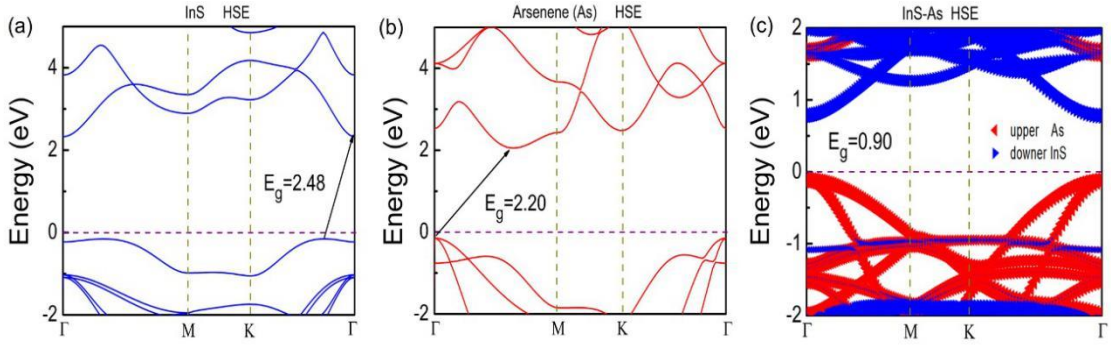


Figure S4. (color online) The projected band structures of InS-As vdWH under finite vertical strains (a) $\Delta d = -0.8\,\mathring{\mathrm{A}}$, (b) $\Delta d = 0.4\,\mathring{\mathrm{A}}$ and (c) $\Delta d = 1.8\,\mathring{\mathrm{A}}$ at HSE level. In each panel, the Fermi level is set to zero.

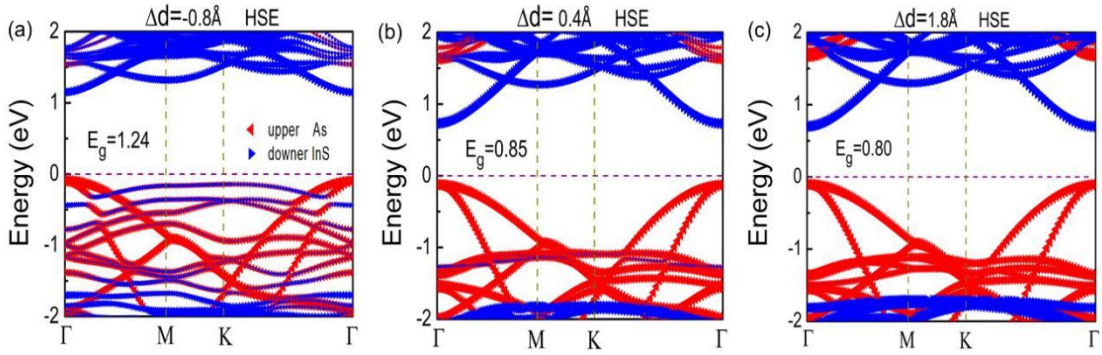


Figure S5. (color online) The projected band structures of InS-As vdWH under finite in-plane strains (a) $\varepsilon = -8\%$, (b) $\varepsilon = 2\%$ and (c) $\varepsilon = 4\%$ at HSE level. In each panel, the Fermi level is set to zero.

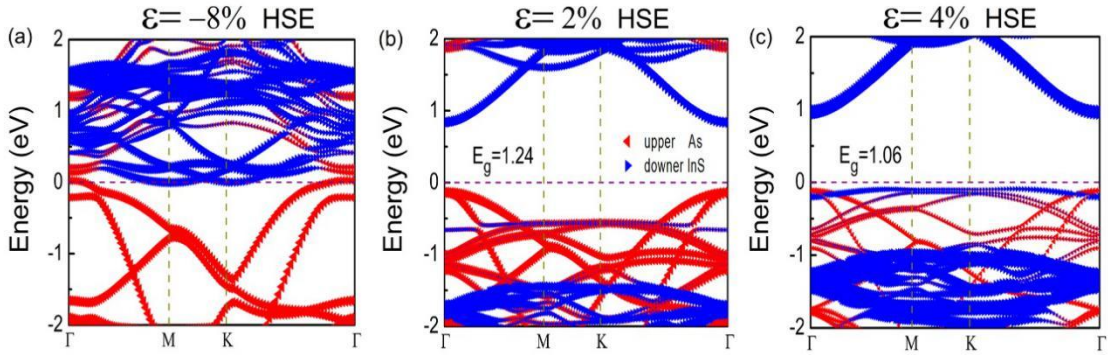


Figure S6. (color online) The projected band structures of InS-As vdWH under finite electric fields (a) $E_{ext} = -0.5V/\mathring{A}$, (b) $E_{ext} = 0.6V/\mathring{A}$ and (c) $E_{ext} = 0.8V/\mathring{A}$ at PBE level and (d) $E_{ext} = -0.8V/\mathring{A}$, (e) $E_{ext} = 0.6V/\mathring{A}$ and (f) $E_{ext} = 0.8V/\mathring{A}$ at HSE level. In each panel, the Fermi level is set to zero.