Supporting Information

Porous Silaphosphorene, Silaarsenene and Silaantimonene: a Sweet Marriage of Si and P/As/Sb

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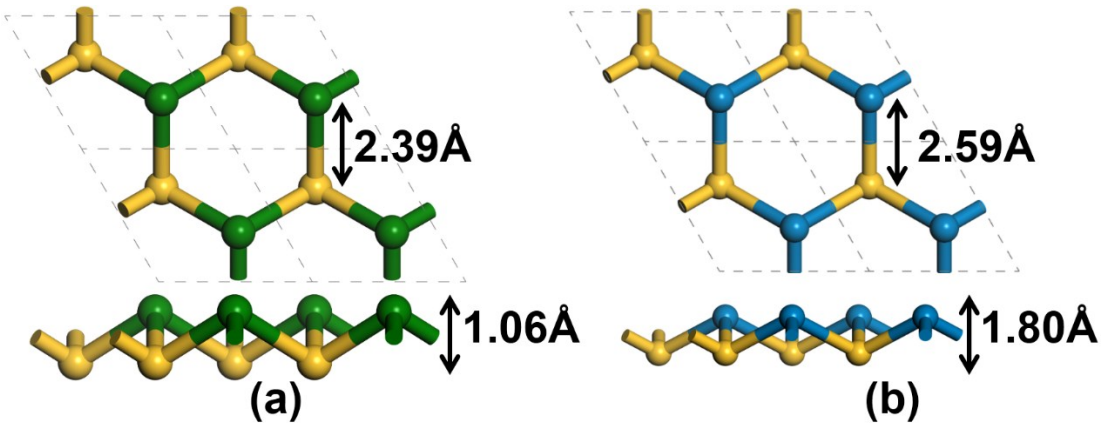

Figure S1. Top and side views of the optimized structures of (a) silicene-like SiAs and (b) silicene-like SiSb monolayers. The green, blue and yellow atoms represent As, Sb and Si atoms, respectively.

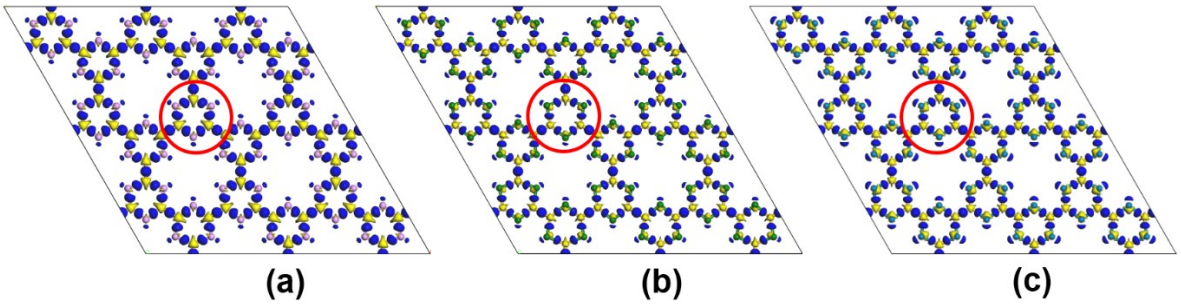

Figure S2. Iso-surface of deformation electronic density of (a) pSiP (0.04 e/au), (b) pSiAs (0.05 e/au) and (c) pSiSb (0.04 e/au). Blue and yellow regions refer to the electron-rich and –deficient regions, respectively.

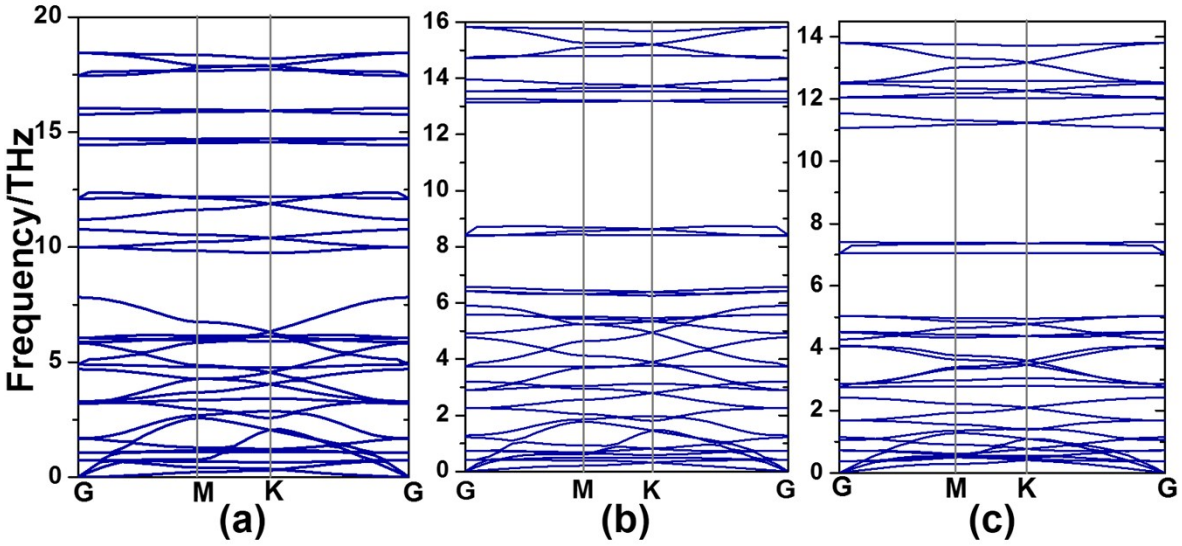

Figure S3. Phonon dispersions of the fully relaxed (a) pSiP, (b) pSiAs and (c) pSiSb monolayers.

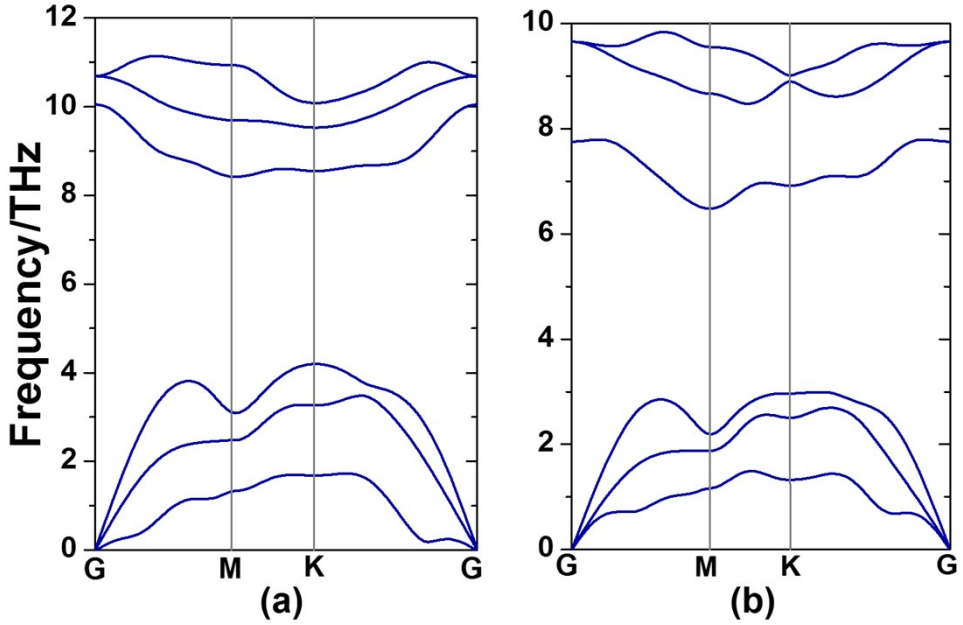

Figure S4. Phonon dispersions of (a) silicene-like SiAs and (b) silicene-like SiSb.

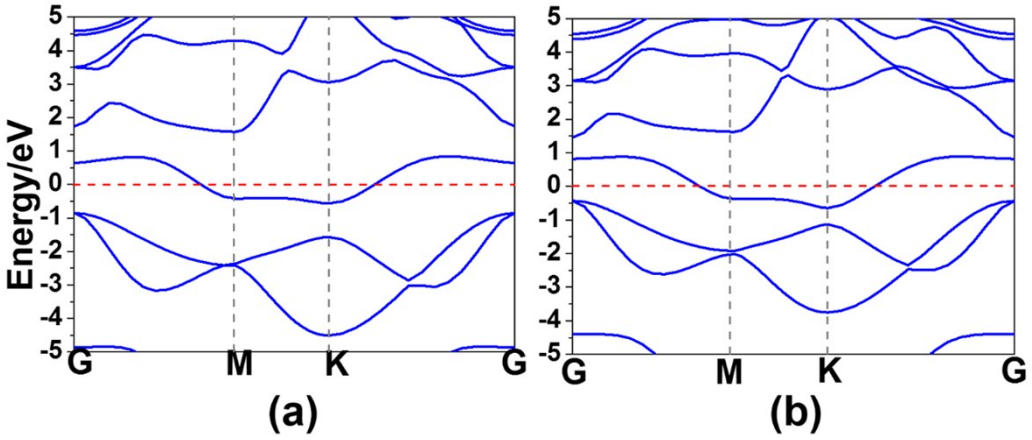

Figure S5. Band structures of (a) silicene-like SiAs and (b) silicene-like SiSb (PBE functional).

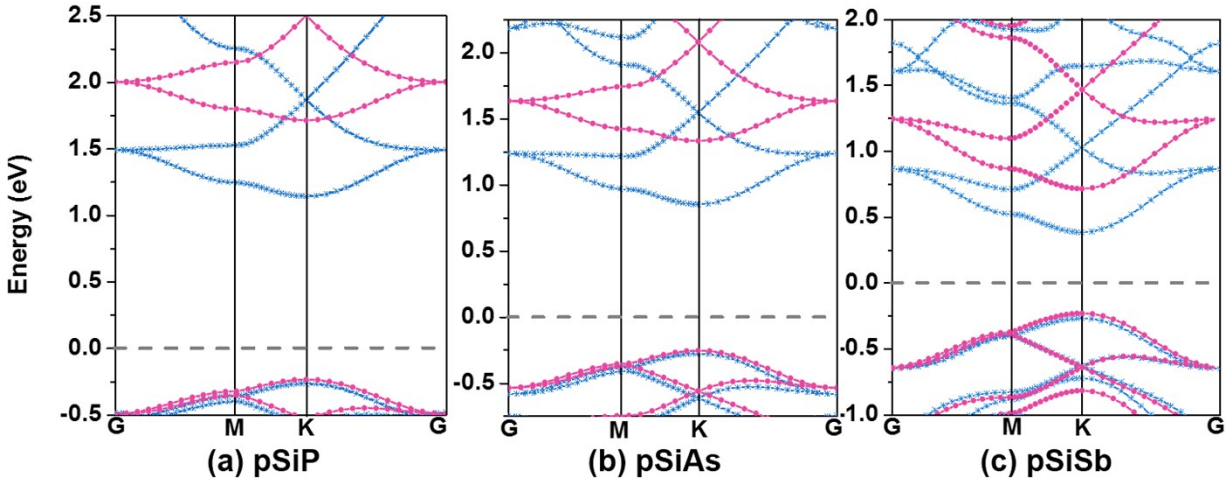

Figure S6. Band structures of (a) pSiP, (b) pSiAs and (c) pSiAs computed at the PBE (the red circle lines) and HSE06 (the blue star lines) level of theory. The dashed gray line indicates the Fermi level.

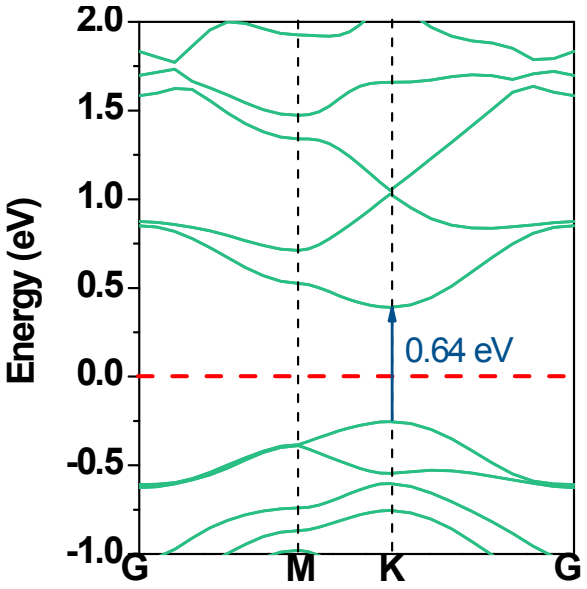

Figure S7. Band structure of pSiSb monolayer including SOC effect (PBE functional).

Table S1. Calculated values of NICS(0) and NICS(1) (ppm) of pnictogen-silicon analogues of benzene.

Molecule	NICS(0)	NICS(1)
$H_3Si_3P_3$ (D_{3h})	-6.26	-6.05
$H_3Si_3As_3$ (D_{3h})	-5.65	-5.65
$H_3Si_3Sb_3$ (D_{3h})	-5.93	-6.25
C_6H_6 (D_{6h})	-8.24	-10.21

In order to evaluate the aromatic character of Si_3P_3, Si_3As_3 and Si_3Sb_3 units, we computed the nucleus independent chemical shift (NICS) values[1] of $H_3Si_3P_3$, $H_3Si_3As_3$ and $H_3Si_3Sb_3$ clusters (Table S1). NICS is a simple and efficient aromaticity probe, and a negative NICS value indicates aromaticity.

$H_3Si_3X_3$ (X=P, As, Sb) molecules were fully optimized by Gaussian 09 program[2] at B3LYP level of theory, 6-31G* basis set was used for H, Si and P, while LANL2DZ basis set was utilized for As and Sb. The NICS values were computed at and 1 Å above the geometric center, which are termed as NICS (0) and NICS (1), by gauge including the atomic orbital (GIAO)[3] method at B3LYP level of theory, 6-311++G(d,p) and LANL2DZ basis sets were used for H/Si/P and As/Sb, respectively.

Though the NICS values of $H_3Si_3P_3$, $H_3Si_3As_3$ and $H_3Si_3Sb_3$ clusters are lower than benzene, their negative values indicate aromatic characters of central Si_3P_3, Si_3As_3 and Si_3Sb_3 units.

(1) P. v. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N. J. v. E. Hommes, *J. Am. Chem. Soc.* 1996, **118**, 6317-8.
(2) Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
(3) R. Ditchfield, *Mol. Phys.* **1974**, *27(4)*, 789-807.