Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2016

Adding a New Dimension to the Chemistry of Phosphorus and Arsenic

Supplemental Information

Li-Ming Yang*[1] and Eric Ganz[2]

[1]*School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, Wuhan 430074, China.*

[2]*Department of Physics, University of Minnesota, 116 Church St., SE, Minneapolis, Minnesota 55416, USA. (email: lmyang.uio@gmail.com)*

Molecular Dynamics (MD) simulations were performed to assess the thermal stability of the Cu_2P and Cu_2As monolayers. For the MD simulations, a 4×4 supercell was used in a $16.06 \times 16.06 \times 13.25$ $Å^3$ box for Cu_2P and a $16.84 \times 16.84 \times 19.40$ $Å^3$ box for Cu_2As.

The detailed parameters are listed in Table S1.

MD Movies are included in the files available for download at temperatures of 300 K, 600 K, 900 K, 1200 K for the last 1 ps of each simulation for Cu_2P and Cu_2As.

Table S1: Comparison of parameters for various Cu_2X materials. Some data included from references S1 and S2.

	Bond Length	**Bond Length Extension**					**Cohesive**	**In Plane**	**Highest Phonon**
		300 K	**600 K**	**900 K**	**1200 K**	**1500 K**	**Energy**	**Stiffness**	**Frequency**
	Å			%			eV	N/m	cm^{-1}
Cu2Si	2.38			16%	37%	Melt	3.46	93	420
Cu2Ge	2.43		17%	30%	40%		3.17	82	320
Cu2As	2.43	18%	36%	Melt	Melt		2.98	82	320
Cu2P	2.33	17%	33%	46%	Melt		3.21	82	400

(S1) Yang, L.-M.; Bačić, V.; Popov, I.; Boldyrev, I.A.; Heine, T.; Frauenheim, T.; Ganz. E. *J. Amer. Chem. Soc.*, **2015**, *137*, 2757

(S2) Yang, L.-M.; Popov, I. A.; Boldyrev, A. I.; Heine, T.; Frauenheim, T.; Ganz, E. *Phys. Chem. Chem. Phys.*, **2015**, *17*, 17545