Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Transition-Metals Decorated Graphdiyne Monolayer as Efficient Sensor toward Phosphide (PH_3) and Arsine (AsH_3)

S. Singsen,[1,2] N. Thasami,[1,3] P. Tangpakonsab,[1,4] H. Bae,[5,6] H. Lee,[5] T. Hussain,[7] T. Kaewmaraya[1,3*]

[1]Department of Physics, Khon Kaen University, Khon Kaen, Thailand

[2]School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

[3]Institute of Nanomaterials Research and Innovation for Energy (IN-RIE), NANOTEC-KKU RNN on Nanomaterials Research and Innovation for Energy, Khon Kaen University, Khon Kaen, 40002, Thailand

[4]Institute of Materials Chemistry, Technische Universität Wien, Getreidemarkt 9/BC/01, 1060 Vienna, Austria

[5]Department of Physics, Konkuk University, Seoul 05029, Republic of Korea

[6]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 7610001, Israel

[7]School of Science and Technology, University of New England, Armidale, New South Wales 2351, Australia

thakaew@kku.ac.th

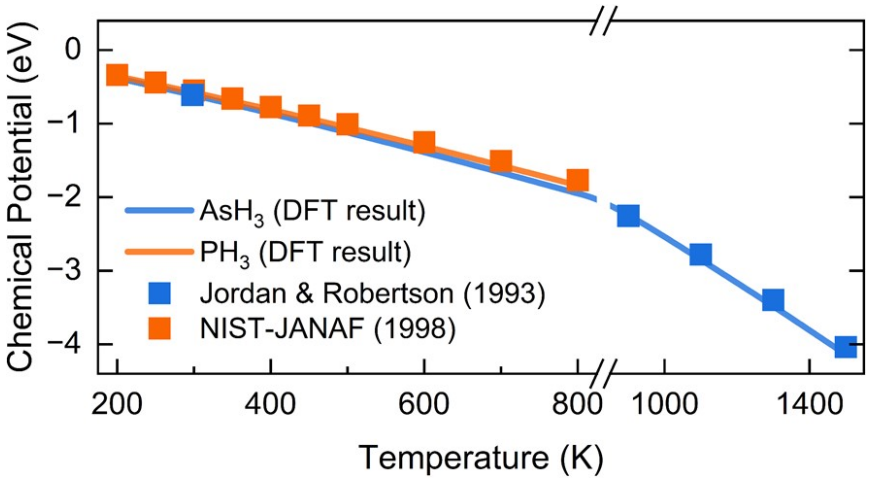

Figure S1. Chemical potential of AsH_3 and PH_3 molecules in the gas phase, calculated in ωB97XD/aug-cc-pVTZ level of theory, and excerpted from experimental reports [1, 2].

References

1. Chase, M.W. and N.I.S. Organization, *NIST-JANAF thermochemical tables*. Vol. 9. 1998: American Chemical Society Washington, DC.
2. Jordan, A. and A. Robertson, *Equilibrium gas-phase composition and thermodynamic properties including subhydrides in the pyrolysis of AsH3 and PH3.* Journal of crystal growth, 1993. **128**(1-4): p. 488-493.