Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Computational design of a novel two dimensional InP nanostructure[1] CONGYAN ZHANG, MING YU, Univ of Louisville — A novel two dimensional (2D) InP nanostructure was predicted through computational simulation on the base of the density functional theory. A monolayer InP sheet was initially designed by substituting indium atoms in phosphorene alternatively. This monolayer InP sheet was then stabilized from the initial puckered honeycomb lattice to a buckled honeycomb lattice with C_{1H} symmetry. Its stability has been confirmed by studying its phonon spectrum. Especially, it was found that its total energy is about 0.09 eV/atom lower than the previously predicted buckled honeycomb InP sheet with C_{3V} symmetry [Phys. Rev. B 80, 155453 (2009)], clearly demonstrating that 2D InP nanostructure will prefer to stay with C_{1H} symmetry. More interestingly, this newly discovered InP sheet possesses semiconducting nature with a direct bandgap of 1.72 eV.

[1]We acknowledge computing resource support from the Cardinal Research Cluster at the University of Louisville.

Congyan Zhang
Univ of Louisville

Date submitted: 08 Nov 2016 Electronic form version 1.4