Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Prediction of Silicon-Based Layered Structures for Optoelectronic Applications WEI LUO, Fudan Univ, YANMING MA, Jilin Univ, XINGAO GONG, HONGJUN XIANG, Fudan Univ, CCMG TEAM — A method based on the particle swarm optimization (PSO) algorithm is presented to design quasi-two-dimensional (Q2D) materials. With this development, various single-layer and bi-layer materials in C, Si, Ge, Sn, and Pb were predicted. A new Si bi-layer structure is found to have a much-favored energy than the previously widely accepted configuration. Both single-layer and bi-layer Si materials have small band gaps, limiting their usages in optoelectronic applications. Hydrogenation has therefore been used to tune the electronic and optical properties of Si layers. We discover two hydrogenated materials of layered Si_8H_2 and Si_6H_2 possessing quasi-direct band gaps of 0.75 eV and 1.59 eV, respectively. Their potential applications for light emitting diode and photovoltaics are proposed and discussed. Our study opened up the possibility of hydrogenated Si layered materials as next-generation optoelectronic devices.

Wei Luo
Fudan

Date submitted: 09 Nov 2014 Electronic form version 1.4