Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Highly Anisotropic intrinsic electronic transport properties of monolayer and bilayer phosphorene from first principles[1] ZHENGHE JIN, JEFFREY MULLEN, KI WOOK KIM, North Carolina State University — We present an analysis of the electron(hole)-phonon scattering in monolayer and bilayer phosphorene using first principles. Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT) are used to calculate the scattering matrix elements and full band Monte Carlo carrier transport simulation is employed to obtain the intrinsic electron/hole mobility. Room temperature mobility and saturation velocity in monolayer and bilayer phosphorene are extracted and significant layer number dependence in the mobility is revealed which results from the carrier-phonon interaction matrix elements. The transport properties are also varied with the crystal orientation with anisotropy mobility mostly attributed to the anisotropic band structure and effective masses. Our calculation reveals monolayer phosphorene has anisotropic hole transport property with the room temperature mobility in the armchair direction (458 cm^2/Vs) about five times larger than in the zigzag direction (90 cm^2/Vs). For bilayer phosphorene, the mobility on both directions increases to 1610 cm^2/Vs and 760 cm^2/Vs along armchair and zigzag direction respectively. The increased mobility in bilayer is consistent with the experiments which revealed low field mobility of over one thousand in multiple layer phosphorene structure, which provides optimal material for channel in field-effect transistor and a good opportunity for high-performance p-type device. [1] This work was supported, in part, by SRC/NRI SWAN.

Jeffrey Mullen
North Carolina State University

Date submitted: 06 Nov 2015 Electronic form version 1.4