Supporting Information

Tunneling transport of 2D anisotropic XC (X = P, As, Sb, Bi) with direct band gap and high mobility: A DFT coupled with NEGF study

Xuemin Hu¹, Wenqiang Liu², Jialin Yang², Wei Wang¹, Luanhong Sun¹, Xiaoqin Shi^{*2}, Yufeng Hao³, Shengli Zhang², Wenhan Zhou^{*2}

¹ School of Material Engineering, Jinling Institute of Technology, Nanjing 211169, China

²Key Laboratory of Advanced Display Materials and Devices, Ministry of Industry and Information Technology, College of Material Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

³ National Laboratory of Solid State Microstructures, College of Engineering and Applied Sciences, Collaborative Innovation Center of Advanced Microstructures, and Jiangsu Key Laboratory of Artificial Functional Materials, Nanjing University, Nanjing 210093, China.

* E-mail: sxq@njust.edu.cn; zhouwenhan@njust.edu.cn



Figure S1. Electron localization function of the α -XC (X = P, As, Sb, Bi) monolayers.



Figure S2. Phonon band dispersions of the (a) PC, (b) AsC, (c) SbC and (d) BiC monolayers, respectively.



Figure S3. Band structures of (a) PC, (b) AsC, (c) SbC and (d) BiC with and without SOC, respectively.



Figure S4. Projected density of states of (a) PC, (b) AsC, (c) SbC and (d) BiC monolayers, respectively.



Figure S5. Iso-surfaces of partial charge densities for the VBM (yellow) and CBM (cyan) of (a) PC, (b) AsC, (c) SbC and (d) BiC monolayers, respectively.