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Field Effect Transistors Based on Phosphorene nanoribbon with Selective Edge-adsorption: A First-principles Study

Mengli Hu¹, Zhixiong Yang², Wenzhe Zhou¹, Aolin Li¹, Jiangling Pan ^{1,a)}, and Fangping Ouyang^{1, 2, a)}

¹School of Physics and Electronics, and Institute of Super-microstructure and Ultrafast Processing Advanced Materials, Central South University, Changsha 410083, People's Republic of China

²Powder Metallurgy Research Institute and State Key Laboratory of Powder Metallurgy, Central South University, Changsha 410083, People's Republic of China

a) Author to whom correspondence should be addressed. Electronic mail: panil@csu.edu.cn and ouyangfp06@tsinghua.org.cn

Abstract: By using density functional theory (DFT) and nonequilibrium Green's function (NEGF), field effect transistors (FET) based on zigzag shaped phosphorene nanoribbons (ZPNR) are investigated. The FETs are constructed with bare-edged ZPNRs as electrodes and H, Cl or OH adsorbed ZPNRs as channel. It is found FETs with the three kinds of channel show similar transport properties. The FET is p-type with a maximum current on/off ratio of 10⁴ and a minimum off-current of 1nA. The working mode of FETs is dependent on the parity of channel length. It can be either enhancement mode or depletion mode and the off-state current shows an even-odd oscillation. The current oscillations are interpreted with density of states (DOS) analysis and methods of evolution operator and tight-binding Hamiltonian. Operating mechanism of the designed FETs is also presented with projected local density of states and band diagrams.

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