Supporting Information for

Black Phosphorus Transistors with van der Waals–type Electrical Contacts

Ruge Quhe,[1] Yangyang Wang,[4] Meng Ye,[2] Qiaoxuan Zhang,[1] Jie Yang,[1] Pengfei Lu,[1] Ming Lei,[1,*] and Jing Lu [2,3,*]

[1]State Key Laboratory of Information Photonics and Optical Communications and School of Science, Beijing University of Posts and Telecommunications, Beijing 100876, P. R. China

[2]State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China

[3]Collaborative Innovation Center of Quantum Matter, Beijing 100871, P. R. China

[4]Nanophotonics and Optoelectronics Research Center, Qian Xuesen Laboratory of Space Technology, China Academy of Space Technology, Beijing 100094, P. R. China

*Corresponding author: jinglu@pku.edu.cn; mlei@bupt.edu.cn

Table S1 Structural parameters of different electrodes. [a]

Electrode	Ni	Gr	Bo	Gr/Ni	BN/Ni
$\bar{\varepsilon}$ (%)	2.45	3.26	3.70	3.05	2.67
d_{min} (Å)	1.45	3.36	3.13	3.03	3.06
h (Å)	2.07	2.09	2.20	2.20	2.19
$d_{P\text{-}P}$ (Å)	2.27	2.24	2.25	2.31	2.31

[a] $\bar{\varepsilon}$: average lattice mismatch; d_{min}: minimum vertical distance from ML BP to adjacent substrate surface; h: average buckling of ML BP; $d_{P\text{-}P}$: average P-P bond length.

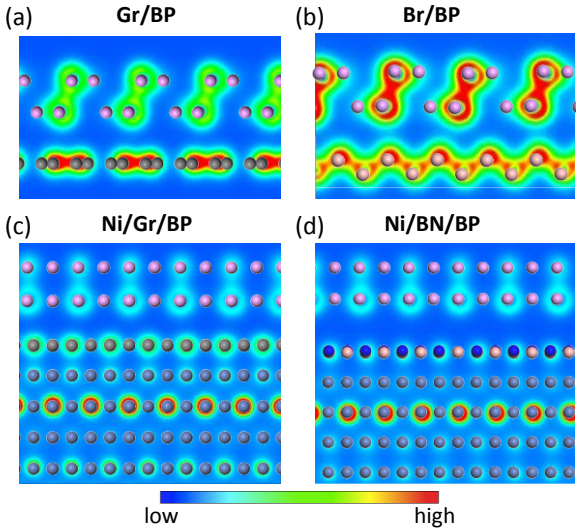

Figure S1 Contour plots of total electron distribution of (a) BP/Gr, (b) BP/Bo, (c) BP/Gr/Ni, and (d) BP/BN/Ni heterostructures. The purple, grey, green, red, and yellow balls represent P, C, B, N, and Ni atoms, respectively.

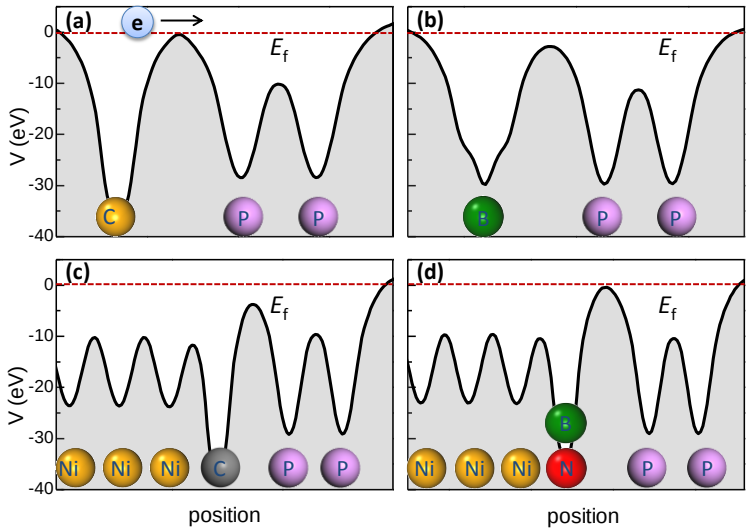

Figure S2 Electrostatic potentials of (a) BP/Gr, (b) BP/Bo, (c) BP/Gr/Ni, and (d) BP/BN/Ni heterostructures along the direction normal to the ML BP surfaces. The dotted line stands for the Fermi level.