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Phosphorene — Metal Contacts YUANYUAN PAN, YANGYANG WANG, MENG YE, RUGE QUHE, HONGXIA ZHONG, ZHIGANG SONG, XIYOU PENG, DAPENG YU, JINBO YANG, State Key Laboratory of Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, LI YANG, Department of Physics, Washington University in St. Louis, St. Louis, Missouri 63130, United States, JING LU, State Key Laboratory of Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China — Recently, phosphorene electronic and optoelectronic prototype devices have been fabricated with various metal electrodes, in which direct contacting with metal electrodes leads to appearance of Schottky barrier at the phosphorene-metal interfaces. In this talk, we will present our new results about the contact properties and Schottky barrier height (SBH) of phosphorene with a series of commonly used metals (Al, Ag, Cu, Au, Cr, Ti, Ni, and Pd) in transistors by using both ab initio electronic structure calculations and more reliable quantum transport simulations. Phosphorene undergoes a metallization under the checked metals, and the metallized phosphorene have an unnegligible coupling with channel phosphorene. The calculated SBHs are in good agreement with the available experimental data with Ni and Ti as electrodes. Our findings not only provide an insight into the phosphorene-metal interfaces but also help in phosphorene based device design.

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