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Supporting Information

Quasiparticle energies and significant exciton effects of monolayered blue arsenic phosphorus conformers

Huiyan Zhao, [a] Qian Wang, [a] Baonan Jia, [a] Lihong Han, [a] Wen Chen,[b] Jinbo Hao, [b] Liyuan Wu*[c], Pengfei Lu*[a] and Pengfei Guan*[d]

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

[b] School of Science, Xi'an University of Architecture and Technology, Xi'an 710055, P. R. China

[c] CAS Key Laboratory for Biomedical Effects of Nanomaterials and Nanosafety, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, P. R. China

[d] Beijing Computational Science Research Center, Beijing 100193, P. R. China

Email: wuly2018@gmail.com; photon.bupt@gmail.com; pguan@csrc.ac.cn

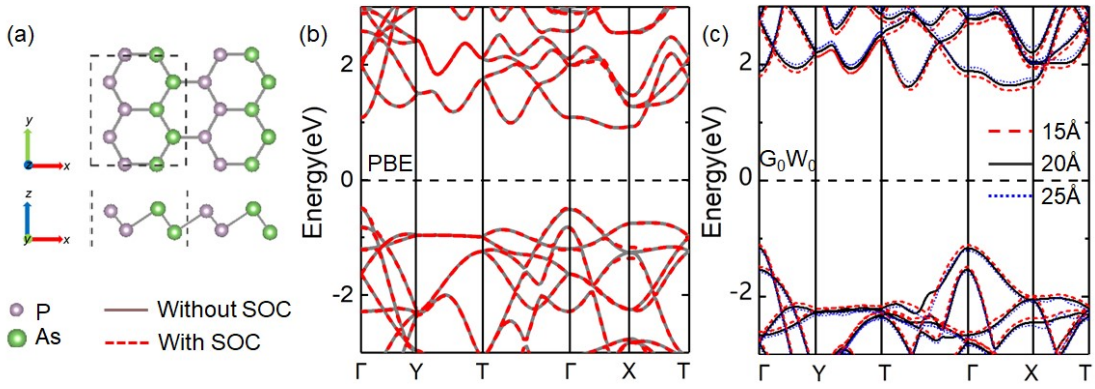

Figure S1 (a) The top and side views of the optimized β_1-AsP. (b) The band structures of β_1-AsP by PBE without SOC (the gray solid lines) and with SOC (the red dotted lines). Taking into account the SOC effect, the bands in the X point show a small spin splitting. The calculated splitting energy of the VBM is about 191 meV. The influence of SOC on the energy band can be ignored. (c) The band structures of β_1-AsP by G_0W_0 with the vacuum layer of 15 Å (the dashed lines), 20 Å (the black solid lines), and 25 Å (the blue dotted lines) with 7×6×1 k-grid. The direct band gaps with the vacuum layer of 15 Å, 20 Å, and 25 Å increase, 2.92, 3.05, and 3.16 eV, respectively. The calculated gaps change between them no more than 250 meV. In our work, we used a vacuum layer of 20 Å in the perpendicular (z) direction to avoid spurious interaction between layers.

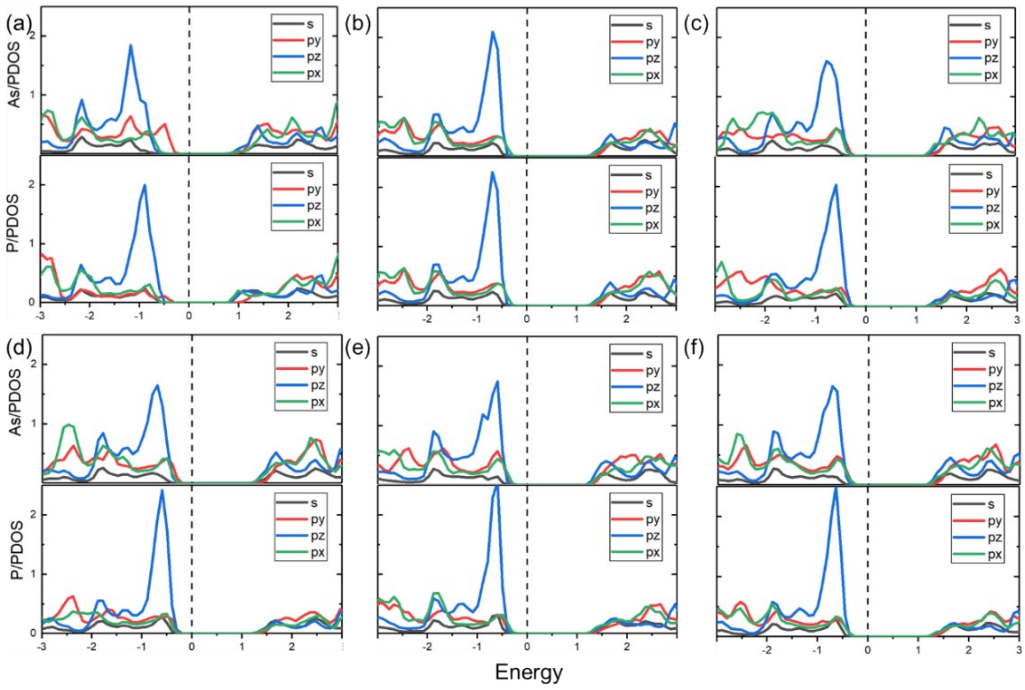

Figure S2 The PDOS with PBE potential for As atoms and P atoms of (a) β_1-AsP, (b) β_2-AsP, (c) β_3-AsP, (d) β_4-AsP, (e) β_5-AsP, and (f) β_6-AsP. Black, red, blue, green lines indicate the *s*, p_y, p_z, p_x orbitals for As or P atoms.