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Many-body Effect, Carrier Mobility, and Device Performance of Hexagonal Arsenene and Antimonene¹ YANGYANG WANG, China Academy of Space Technology, MENG YE, Peking University, RUGE QUHE, Beijing University of Posts and Telecommunications, PU HUANG, JING LU, Peking University — Monolayer (ML) arsenene and antimonene, as new members of group V-enes, have attracted great interest. Experimentally, multilayer arsenene/antimonene nanoribbons have been fabricated on an InAs/InSb substrate. ML and multilayer antimonene have been isolated by mechanical exfoliation and liquid-phase exfoliation. More importantly, they are highly stable under ambient condition. Together with their wide band gaps predicted by the HSE theory, arsenene and antimonene are very attractive for nanoscale optoelectronic and electronic devices. We investigate the many-body effect and device performance of ML hexagonal arsenene and antimonene using ab initio GW, GW plus Bethe-Salpeter equation and nonequilibrium Green's function approach. The quasi-particle and optical band gaps are calculated in ML arsenene and antimonene for the first time. Low $(21/66 \text{ cm}^2/\text{V} \cdot \text{s})$ for electron/hole) and moderate carrier mobilities $(150/510 \text{ cm}^2/\text{V} \cdot \text{s} \text{ for electron/hole})$ are obtained, for arsenene and antimonene, respectively. Quantum transport simulation reveals that the performance limits of sub-10 nm ML arsenene and antimonene FETs can satisfy both low power and high performance requirements of the ITRS target in the next decade.

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