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Optical properties of single and bilayer arsenene phases[1] DENIZ KECIK, SALIM CIRACI, ENGIN DURGUN, Bilkent University - UNAM — An extensive investigation of the optical properties of single-layer buckled and washboard arsenene and their bilayers was performed, starting from layered three-dimensional (3D) crystalline phase of arsenic using density functional and many-body perturbation theories combined with Random Phase Approximation. Electron-hole interactions were taken into account by solving the Bethe-Salpeter equation, suggesting first bound exciton energies on the order of 0.7 eV. Thus, many-body effects were found to be crucial for altering the optical properties of arsenene. The light absorption of single layer and bilayer arsenene structures in general falls within the visible-ultraviolet (UV) spectral regime. Moreover, directional anisotropy, varying the number of layers and applying homogeneous or uniaxial in-plane tensile strain were found to modify the optical properties of two-dimensional (2D) arsenene phases, which could be useful for diverse photovoltaic and optoelectronic applications.

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