STRONG EXCITONS IN HYDROGENATED TWO-DIMENSIONAL GROUP-IV CRYSTALS: GRAPHANE, POLYSILYNE AND POLYGERMYNE

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Using a combination of the GW quasiparticle theory and the solution of the electron-hole Bethe-Salpeter equation, excitonic pair excitations and optical properties of group IV sheets are studied from first principles. We demonstrate that the hydrogen-passivated sheet crystals of carbon[1], silicon, and germanium overcome the limitations, for optical applications, of the corresponding indirect gap 3D semiconductors and of their zero gap 2D allotropes graphene, silicene[2], and germene. This holds especially for the quasi direct gaps Si- and Ge-derived 2D systems. The extremely large exciton binding energies of 1.8, 0.9, or 0.6 eV and strong oscillator strengths make them interesting candidates for optoelectronics in the blue-green region.

References

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