Two-Dimensional 2γ-In2Se$_3$ in Bilayer-like Coloring Triangle Lattice: Mechanical, Electronic, Transport, and Photocatalytic Properties

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The discovery of two-dimensional (2D) materials derived from non-van der Waals (vdW) bulk counterparts has opened up a new era, drawing attention to the crystals composed of asymmetrically bonded vertical exotic layers. In this respect, γ-In_2Se_3,[1] a promising material utilized in various applications, built with coloring triangle layers, emerges as a suitable candidate. Through first-principles calculations, we show that a novel 2D structure, the 2γ-In_2Se_3 monolayer, consisting of a bilayer-like coloring triangle lattice, can be exfoliated from bulk γ-$In_2Se_3$with minimal external energy. The crystal structure prediction of this monolayer is also performed using the particle swarm-optimization method [2]. The formation of this exotic 2D lattice is facilitated by sp^3 hybrid bonds. Comprehensive phonon dispersion and finite-temperature molecular dynamics analyses confirm the thermodynamic stability of the 2γ-In_2Se_3 monolayer. The material exhibits an anisotropic mechanical response due to missing bonds at lattice sites, making it suitable for flexible nanoelectronic devices. It possesses semiconductor characteristics with an indirect bandgap in the visible region. Analysis of band edge positions and charge carrier mobility suggests that the 2γ-In_2Se_3 monolayer is highly efficient for photocatalytic water-splitting applications [3].

References

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Figures

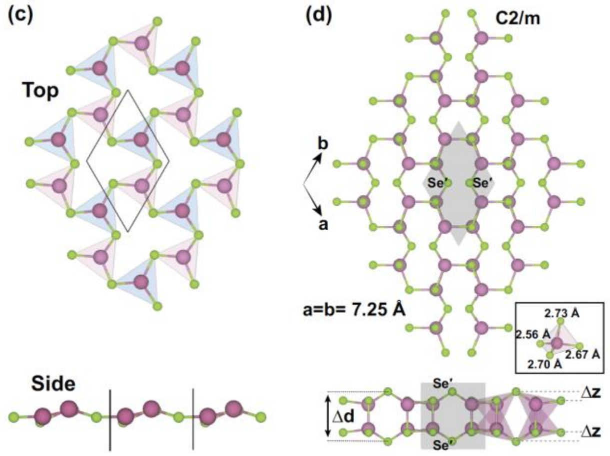

Figure 1. (c) Top and side views of the deformed coloring triangle lattice of a single layer of γ-In_2Se_3, with the unit cell delineated. (d) Top and side views of the bilayer-like coloring triangle lattice of the 2γ-In_2Se_3 monolayer in the C2/m space group. The unit cell is shaded, and the two-fold coordinated Se′ atoms are indicated.