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Few-layer Tellurium: one-dimensional-like layered elementary semiconductor with striking physical properties

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Abstract

Few-layer Tellurium, an elementary semiconductor, succeeds most of striking physical properties that black phosphorus (BP) offers and could be feasibly synthesized by simple solution-based methods. It is comprised of non-covalently bound parallel Te chains, among which covalent-like feature appears. This feature is, we believe, another demonstration of the previously found covalent-like quasi-bonding (CLQB) where wavefunction hybridization does occur. The strength of this inter-chain CLQB is comparable with that of intra-chain covalent bonding, leading to closed stability of several Te allotropes. It also introduces a tunable bandgap varying from nearly direct 0.31 eV (bulk) to indirect 1.17 eV (2L) and four (two) complex, highly anisotropic and layer-dependent hole (electron) pockets in the first Brillouin zone. It also exhibits an extraordinarily high hole mobility (~10⁵ cm²/Vs) and strong optical absorption along the non-covalently bound direction, nearly isotropic and layer-dependent optical properties, large ideal strength over 20%, better environmental stability than BP and unusual crossover of force constants for interlayer shear and breathing modes. All these results manifest that the few-layer Te is an extraordinary-high-mobility, high optical absorption, intrinsic-anisotropy, low-cost-fabrication, tunable bandgap, better environmental

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