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Structural and electronic properties of atomically thin germanium selenide polymorphs ZIYU HU, Beijing Computational Science Research Center — Using comprehensive density functional theory calculations, we systematically investigate the structure, stability, and electronic properties of five polymorphs of GeSe monolayer, and highlight the differences in their structural and electronic properties. Our calculations show that the five free-standing polymorphs of GeSe are stable semiconductors. β-GeSe, γ-GeSe, δ-GeSe, and ε-GeSe are indirect gap semiconductors, whereas α-GeSe is a direct gap semiconductor. We calculated Raman spectra and scanning tunneling microscopy images for the five polymorphs. Our results show that the β-GeSe monolayer is a candidate for water splitting.

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