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**Single layer lead iodide: computational exploration of structural, electronic and optical properties, strain induced band modulation and the role of spin-orbital-coupling** MEI ZHOU, WENHUI DUAN, Department of Physics and State Key Laboratory of Low-dimensional Quantum Physics, Tsinghua University, Beijing 100084, China, YING CHEN, Institute for Frontier Materials, Deakin University, Waurin Ponds, VIC 3216, Australia, AIJUN DU, School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD 4001, Australia — Graphitic like layered materials exhibit intriguing electronic structures and the search for new types of two-dimensional (2D) monolayer materials is of great interest for developing novel nano-devices. By using density functional theory method, we investigate the structure, stability, electronic and optical properties of monolayer lead iodide ( $\text{PbI}_2$ ). The stability of  $\text{PbI}_2$  monolayer is first confirmed by phonon dispersion calculation. Compared to the calculation using generalized gradient approximation, screened hybrid functional and spin-orbit coupling effects can predicts an accurate band gap (2.63 eV). The biaxial strain can tune its band gap size in a wide range from 1 eV to 3 eV, which can be understood by the strain induced uniformly change of electric field between Pb and I atomic layer. The calculated imaginary part of the dielectric function of 2D graphene/ $\text{PbI}_2$  van der Waals type hetero-structure shows significant red shift of absorption edge compared to that of a pure monolayer  $\text{PbI}_2$ . Our findings highlight a new interesting 2D material with potential applications in nanoelectronics and optoelectronics.

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