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Electronic and Optical Properties of Atomically Thin PbI_2 Crystals ALEXIS TOULOUSE, BENJAMIN ISAACOFF, Physics, University of Michigan, GUANGSHA SHI, Materials Science and Engineering, University of Michigan, MARIE MATUCHOVÁ, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, ROBERTO MERLIN, Physics, University of Michigan — Layered materials with weak inter-layer van der Waals bonds such as PbI_2 are of interest for the novel properties they can exhibit as their thickness is reduced to the monolayer limit. We present the results of a joint experimental and theoretical study of the optical and electronic properties of atomically thin samples of PbI_2. First-principles calculations based on density functional and many-body perturbation theory were performed for the electronic, excitonic, and optical properties of mono and few-layer structures. These results are compared with emission data from photoluminescence experiments performed on mechanically exfoliated samples ranging from bulk to a few monolayers. Our results show that despite a significant increase in the electronic band gap due to quantum confinement in ultrathin samples, the optical gap, defined by excitonic effects, remains unaffected by quantum confinement until its dimensions are reduced to one monolayer. Computational resources were provided by the DOE NERSC facility.

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