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**Optoelectronic and transport properties of epitaxially strained $BiVO_4$ from first principles** SEBASTIAN E. REYES-LILLO, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley, JEFFREY B. NEATON, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley; Kavli ENSI — Bismuth vanadate ($BiVO_4$) is a promising photo-catalyst for water-splitting. However, the photo-electrochemical performance of $BiVO_4$ is limited by a relatively large band gap ($\sim$2.5eV) and low electron mobilities. Previous theoretical work has focused on the role of extrinsic and intrinsic defects to control and tune the optical and transport properties of $BiVO_4$; however, the effect of anisotropic strain remains largely unexplored. Recently, thin films $BiVO_4$ have been grown using molecular beam epitaxy, opening new possibilities to design $BiVO_4$-based renewable solar-energy devices. In this work, we use density functional theory and GW/BSE many-body perturbation theory calculations to investigate the effect of epitaxial strain in the structural, optoelectronic and transport properties of $BiVO_4$. We find that compressive epitaxial strain leads to a moderate decrease of the band gap and an enhancement of hole effective mass and majority carrier small polaron formation energy. In addition, we determine the effect of epitaxial strain on the transport properties of electron and hole polarons and their interaction with oxygen vacancies. This work is supported by DOE, computational resources are provided by NERSC.

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