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**Quasiparticle and optical band gaps of $Sr_{n+1}Ti_nO_{3n+1}$ from *ab-initio* many-body perturbation theory** SEBASTIAN E REYES-LILLO, TONATIUH RANGEL, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley, FABIEN BRUNEVAL, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley; CEA, DEN, SRMP , JEFFREY B NEATON, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley; Kavli ENSI — The Ruddlesden Popper homologous series $Sr_{n+1}Ti_nO_{3n+1}$ provides a unique opportunity to study the effect of dimensionality and confinement on the band gap and absorption spectrum of the complex oxide $SrTiO_3$. In this work, we use many-body perturbation theory within the $GW$ approximation and the Bethe-Salpeter equation (BSE) approach to study the electronic and optical properties of $Sr_{n+1}Ti_nO_{3n+1}$. We find that our $GW$/BSE direct and indirect band gaps are in excellent agreement with measured direct and indirect optical gaps. We discuss technical aspects of the calculations such as convergence and starting-point dependence, and compare to higher levels of theory. In addition, we find a relatively large exciton binding energy of 500 meV for $Sr_2TiO_4$ ($n = 1$). We explore the role of structural distortions and epitaxial strain in the properties of the localized exciton. Our work suggests that layered structures can provide a viable route for the design of complex oxide materials with desirable optoelectronic properties. This work is supported by DOE.

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