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Ab-Initio Study of Excitonic Absorption for Layered LaCuChO and BaCuChF (Ch={S,Se,Te}) Structures JASON VIELMA, GUENTER SCHNEIDER, Oregon State University — Layered oxychalcogenides LnCuChO (Ln = {La,Pr,Nd}, Ch = {S,Se,Te}) and isostructural layered fluorochalcogenides BaCuChF have drawn much interest in recent years as p-type wide bandgap semiconductors with applications in transparent electronics and photovoltaics. Members of both materials show strong excitonic absorption, which is observable at room temperature. However, recent studies disagree on the origin and nature of the room temperature excitons in the respective families of materials, with Ueda et al. [1] attributing the room temperature excitonic absorption in LaCuSeF to 2 dimensional quantum confinement of hole carriers in the layered structure, while Zakuatyev et al. [2] argue that the room temperature excitonic absorption in BaCuChF is well described by a 3 dimensional Wannier-Mott excitonic model. We report an ab-initio computational study of the optical properties including the excitonic effects for both families of materials. The optical properties are calculated using the Bethe-Salpeter equation in the GW approximation.

[1] K. Ueda, et al. *Phys. Rev. B*, **69** 155305 (2004).
[2] A. Zakutayev, et al. *Phys. Rev. B*, **81** 155103 (2010).

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