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Optical properties of 2D monochalcogenides: single-layer GaSe and GaTe from first-principles calculations[1] GABRIEL ANTONIUS, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Two-dimensional (2D) metal monochalcogenides such as gallium selenide and gallium telluride show good electrical properties, and an exceptionally large photoresponsitivity, making it suitable for photodetectors and phototransistor devices. We compute the absorption spectrum of single-layer GaSe and GaTe from first-principles calculations, using the GW and BSE formalism. The hydrogenic series of bound excitons (derived from the lowest interband transition) found in these materials is dark in linear optical response, due to the different symmetry of the first valence and conduction band. The high-energy bright excitons assume a non-hydrogenic behavior located neither in the center nor the boundary of the Brillouin zone, where a high density of states allows for large absorbance.

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