Electronic bandgap and exciton binding energy of layered semiconductor TiS₃

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We present a study of the electronic and optical bandgap in layered TiS_3 , an almost unexplored semiconductor that has attracted recent attention because of its large carrier mobility and inplane anisotropic properties, to determine its exciton binding energy.¹⁻⁴ We combine scanning tunneling spectroscopy and photoelectrochemical measurements with random phase approximation and Bethe-Salpeter equation calculations to obtain the electronic and optical bandgaps and thus the exciton binding energy. We find experimental values for the electronic bandgap, optical bandgap and exciton binding energy of 1.2 eV, 1.07 eV and 130 meV (Fig. 1), respectively, and 1.15 eV, 1.05 eV and 100 meV for the corresponding theoretical results. The exciton binding energy is orders of magnitude larger than that of common semiconductors and comparable to bulk transition metal dichalcogenides, making TiS₃ ribbons a highly interesting material for optoelectronic applications and for studying excitonic phenomena even at room temperature.

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Figure 1. a) Colormap histogram of STS current-voltage curves (current in absolute value). A representative current-voltage curve is plotted in solid black line. Inset: AFM topographic image of TiS_3 ribbons. b) Photocurrent density as a function of light wavelength (energy). The optical bandgap energy is determined by the point where the linear fit cuts the zero photocurrent density (highlighted in the inset).