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Quasiparticle and Optical Properties of Mono- and Bi-layer SnS2: A First-Principles GW and GW+BSE Study[1] MENG WU, DIANA QIU, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Unlike most semiconducting transition metal dichalcogenides, SnS2, another layered metal dichalcogenide, is calculated within density functional theory to be an indirect bandgap semiconductor in both its bulk and monolayer forms. Experimental characterization of mono- and bi-layer SnS2 has been performed, but the details of its quasiparticle and excitonic properties remain unclear. Thus, we employ ab initio GW and GW+BSE calculations to study the quasiparticle band structure and optical absorption spectrum, respectively, of mono- and bi-layer SnS2 with spin-orbit coupling included throughout the calculations. We further investigate the character of excitonic states contributing to the optical spectrum.

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Meng Wu
Physics Department, UC Berkeley and Lawrence Berkeley National Lab

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