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Lateral Heterostructures of Monolayer Transition Metal Dichalcogenides: a First-principles Study[1] MENG WU, TING CAO, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Using first-principles calculations, we investigate the electronic structure and optical properties of lateral heterostructures consisting of different monolayer transition metal dichalcogenides (TMDs). We find that the spin-orbital coupling effect plays an important role in modifying the ground-state electronic structure and excited-state properties such as optical responses. The anisotropy of optical absorption is investigated including local-field effects.

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

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