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Indirect Band Gap Emission by Hot Electron Injection in Metal/MoS_2 and Metal/WSe_2 Heterojunctions ZHEN LI, University of Southern California, GOUTHAM EZHILARASU, College of Engineering Guindy, Anna University, IOANNIS CHATZAKIS, ROHAN DHALL, CHUN-CHUNG CHEN, STEPHEN CRONIN, University of Southern California — Transition metal dichalcogenides (TMDCs), such as MoS_2 and WSe_2, are free of dangling bonds, therefore make more "ideal" Schottky junctions than bulk semiconductors, which produce recombination centers at the interface with metals, inhibiting charge transfer. Here, we observe a more than 10X enhancement in the indirect band gap PL of TMDCs deposited on various metals, while the direct band gap emission remains unchanged. We believe the main mechanism of light emission arises from photoexcited hot electrons in the metal that are injected into the conduction band of MoS_2 and WSe_2, and subsequently recombine radiatively with minority holes. Since the conduction band at the K-point is 0.5eV higher than at the Σ-point, a lower Schottky barrier of the Σ-point band makes electron injection more favorable. Also, the Σ band consists of the sulfur p_z orbital, which overlaps more significantly with the electron wavefunctions in the metal. This enhancement only occurs for thick flakes, and is absent in monolayer and few-layer flakes. Here, the flake thickness must exceed the depletion width of the Schottky junction, in order for efficient radiative recombination to occur in the TMDC. The intensity of this indirect peak decreases at low temperatures.

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