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A unified understanding of the thickness-dependent bandgap transition in hexagonal layered semiconductors JOONGOO KANG, DGIST, Deagu 711-873, Korea, LIJUN ZHANG, Jilin University, Changchun 130012, China, SU-HUAI WEI, Beijing Computational Science Research Center, Beijing 100094, China — Over the past few years, it has been recognized that a single layer of hexagonal two-dimensional semiconductors—such as hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDs)—has a direct bandgap, while it becomes an indirect semiconductor as the number of layers increases to two or more. Understanding and control of the direct-to-indirect bandgap transition (DIBT) of hexagonal layered semiconductors is of great scientific and technological importance, because the DIBT converts multilayer hBN or TMD into optically less active materials. Here, taking hBN and MoS_2 as examples, we provide a microscopic understanding of the DIBT of hexagonal layered semiconductors based on our symmetry analysis and direct first-principles calculations. Starting from a simple phenomenological explanation of the DIBT within the first-order perturbation theory of multilayer phases, we show how the bandgap transition arises from the selective orbital couplings in hexagonal layered semiconductors.

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