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Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides BING HUANG, Beijing Computational Science Research Center, MINA YOON, BOBBY SUMPTER, Oak Ridge National Lab, SUHUAI WEI, Beijing Computational Science Research Center, FENG LIU, University of Utah — Developing practical approaches to effectively reduce the amount of deep defect levels in semiconductors is critical for their use in electronic and optoelectronic devices, but this still remains a very challenging task. In this talk, we propose that specific alloying can provide an effective means to suppress the deep defect levels in semiconductors while maintaining their basic electronic properties. Specifically, we demonstrate that for transition-metal dichalcogenides, such as MoSe2 and WSe2, where anion vacancies are the most abundant defects that can induce deep levels, the deep levels can be effectively suppressed in MoWSe2 alloys at low W concentrations. This surprising phenomenon is associated with the fact that the band edge energies can be substantially tuned by the global alloy concentration, whereas the defect level is controlled locally by the preferred locations of Se vacancies around W atoms. Our findings illustrate a concept of alloy engineering and provide a promising approach to control the defect properties of semiconductors.

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