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Band gap bowing in large size-mismatched II-VI alloys¹ SU-HUAI WEI, CHANG-YOUN MOON, National Renewable Energy Laboratory, Y.Z. ZHU, G.D. CHEN, Xian Jiaotong University — Band gap bowing coefficients in large size-mismatched II-VI alloys $M^{II}X_{1-x}^{VI}O_x$ with $M^{II}=\text{Zn}$ and Cd , and $X^{VI}=\text{S}$, Se , and Te in the zinc-blend structure are calculated using first-principles methods. We show that in these systems, the bowing coefficients are large and composition-dependent. The bowing coefficients increase as the size and chemical mismatch between the constituents increase. The bowing coefficients for the Zn alloys are larger than the corresponding Cd alloys, but smaller than the corresponding III-V alloys. We show that these results can be explained by the size and atomic eigenvalue differences between the constituents and the resulting band offsets and isovalent defect levels in these systems. Our results are compared with recent experimental data.

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