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**Transition-metal impurities and intercalation in $Bi_2Se_3$** M. WEINERT, Y. LIU, L. LI, U. Wisconsin-Milwaukee — The prototype topological insulator $Bi_2Se_3$ consists of 5-layer (QL) units. Using first-principles calculations, we show that even for large (20%) elongations along the c-axis, the in-plane lattice constant remains essential unchanged and the nearest neighbor bond lengths within a QL vary by only $\sim$0.02 Å. These results suggest that impurities may preferentially intercalate between the QLs, possibly leading to $\delta$-doped topological insulator superlattices. For Cu-intercalated $Bi_2Se_3$, the calculated separation between QLs slightly contracts ($\sim$2%), and the Cu intercalation layer provides the internal surfaces necessary for the material to exhibit a Dirac cone. The competition between substitutional impurities and intercalation layers for Cu and Mn will be discussed and compared to experiment.

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