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Tuning the vertical location of topological surface states in ZnSe/Bi_2Se_3 heterostructures via the ZnSe overlayer thickness[1]
LEIQIANG LI, GUANGFEN WU, JIANG ZENG, WEI QIN, PING CUI, ZHENYU ZHANG, Univ of Sci & Tech of China — The robust metallic topological surface states (TSSs) of topological insulators (TI) have attracted intensive research interest both fundamentally and for their potential applications. The precise location of the TSSs defines the boundary between the TI and topologically inequivalent system such as a conventional insulator (CI).[2] Here, by employing first-principles density functional theory calculations, we study the prototype systems of ZnSe/Bi_2Se_3 heterostructures to reveal accurate tunability of the vertical location of the TSSs. We show that the TSSs float to the top of the ZnSe overlayer when its thickness is 1 or 2 monolayers, but are pushed down into the TI when the overlayer is thicker. We further investigate how the atop TSSs may serve as an electron bath in enhancing the catalytic activity of the ZnSe overlayer, using CO oxidation as a test case and paying particular attention to the effects of spin-orbit coupling.[3]

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[2]G. Wu *et al.*, Sci. Rep. **3**, 1233 (2013)
[3]H. Chen *et al.*, Phys. Rev. Lett. **107**, 056804 (2011)

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