Precise Control of the Electronic Structure in AB_2C_4-Type Topological Compounds

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Magnetic topological insulators of the $MnBi_2Te_4$ family (AB_2C_4-type) have recently attracted significant attention due to the possibility of realizing exotic states such as the quantum anomalous Hall effect, axion electrodynamics, and Weyl semimetal phases. A key challenge for their practical implementation in quantum and spintronic technologies is the precise control of their electronic structure, including smooth modification of the bulk gap and topological surface states [1]. An effective strategy to achieve this control is chemical substitution, which enables systematic tuning of band topology and electronic properties. In this work we demonstrate that targeted substitution at different lattice sites (Mn → Pb, Bi → Sb, Te → Se) provides versatile means for engineering the electronic structure of AB_2C_4-type compounds. To reveal the underlying mechanisms, we investigated these systems using angle-resolved photoemission spectroscopy (ARPES), including photon-energy dependence, spin-resolved, and circular dichroism measurements.

For $(Mn_{1-x}Pb_x)Bi_2Te_4$, ARPES revealed a gradual reduction of the bulk band gap with Pb substitution, its closure near $x \approx 40\%$, and reopening above $x \approx 80\%$, consistent with a topological phase transition. Topological surface states are present at low and high Pb concentrations, but vanish near 50–60%, where the system becomes trivial or semimetallic [2]. The type of antiferromagnetic order remains unchanged, while the Néel temperature decreases with Mn dilution [3]. In the $(Mn,Pb)Bi_2Te_4$ system, additional Bi → Sb substitution leads to a controlled shift of the Fermi level, allowing tuning of carrier concentration. The amount of Sb required to reach a compensated semiconductor state depends on the Pb content. For $GeBi_2Te_4$ and $SnBi_2Te_4$, Te → Se substitution systematically modifies the bulk band gap, conduction band dispersion, and topological surface state group velocity. Differences between Ge- and Sn-based systems reflect cation site occupation and disorder, which affect scattering and transport.

Overall, our results demonstrate that controlled substitution in AB_2C_4-type compounds is an effective route for precise tuning of their electronic, magnetic, and topological properties. This chemical flexibility enables the design of materials with tailored phases, opening new opportunities for spintronic and quantum applications.

Bibliography

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