Topology of Hg-based chalcogenides – ab intio studies

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The research on topological materials emerges as one of the most active fields in the condensed matter physics. We have investigated the electronic topological properties of the bulk and interface of Hg-based chalcogenide materials (HgX, X=S, Se, Te) by means of the density functional theory. To have a better insight on the topological properties of the interface, we have studied the electronic band structure at the interface between these materials and the trivial insulator CdTe. The Weyl semimetal phase is found for such interfaces. Furthermore, we have examined the interface between different Hg-based chalcogenides. Finally, we have investigated the effect of strain demonstrating significant changes of the topological properties.