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Relativistic effects in HgTe and CdTe electronic structures

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Quantum spin Hall phase, or also referred as Topological Insulator state, has been obtained in 2007 in a CdTe/HgTe quantum well [1]. These novel state is possible due to the inverted band order near the Fermi energy. These behaviour is originated because there exist a non negligible correlation between valence electrons of the 5d- and 6s-orbital of Hg [2], and relativistic effects [3], specifically spin-orbit coupling [4].

In this work, we present the electronic structure of Cadmium Telluride (CdTe) and Mercury Telluride (HgTe), obtained using the local spin density approximation, including the Hubbard correction (LSDA+U), in the density functional theory (DFT), considering non relativistic, relativistic, and relativistic with spin-orbit coupling effects for each alloy. The results show that relativistic effects reduce the band gap for materials alloys, and inverted band ordering for HgTe is only possible if spin-orbit coupling is considered.

References

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Primary author(s): Mr HINOSTROZA VARGAS MACHUCA, Cristhian David (Universidad Nacional Mayor de San Marcos)

Co-author(s): Dr RIVERA RIOFANO, Pablo Hector (Universidad Nacional Mayor de San Marcos)

Presenter(s): Mr HINOSTROZA VARGAS MACHUCA, Cristhian David (Universidad Nacional Mayor de San Marcos)

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