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Effect of strain on electronic structure and thermoelectric property of a Bi₂Te₃/Sb₂Te₃ compound

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Compounds of bismuth telluride and antimony telluride have greatly attracted the attention of researchers in the years due to the potential applications in the fields of thermoelectrics and spintronics. In this work, we present first-principles calculation of a compound of bismuth telluride - antimony telluride using Quantum Espresso package within the framework of density functional theory. The results of electronic structure calculation show degenerate valleys at the band edges suggesting an enhancement of the power factor by band engineering. To substantiate, we use the solution of semi-classical Boltzmann's equation in a constant relaxation-time approximation to compute the transport coefficients, i.e. the Seebeck coefficient, the electrical conductivity, and the power factor. We demonstrate that the band topology near Fermi energy is tunable under the effects of strain which impacts efficiently on the transport property of the compound. The results suggest a promising technique to improve thermoelectric performance of the compound.

Presenter: Tran Van Quang

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Excitonic condensation phase diagram in the extended Falicov-Kimball model with electron-phonon interaction

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Influence of temperature on the excitonic condensation state in two-dimensional extended Falicov-Kimball model with electron-phonon interaction has been investigated by using the unrestricted Hartree-Fock approximation. Treating both the Coulomb interaction and the electron-phonon coupling in an equal footing, we analyze phase diagrams of the excitonic condensation state. At a given electron-phonon coupling, lowering temperature we find out a semimetal-excitonic condensate at a small Coulomb interaction and a semiconductor-excitonic condensate at a large Coulomb interaction. The excitonic condensate window is enlarged if the electron-phonon coupling is increased. A crossover from a BCS type to a BEC type of the excitonic condensation state driven either by the Coulomb interaction or the electron-phonon coupling in this systems at low temperature is also addressed.

Presenter: Do Thi Hong Hai

P.72 – Poster, NCTP-42

Production and decay of Higgs in the Randall-Sundrum model at high energy colliders

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