Unveiling quantum phase transition by disorder and defects in 2D-materials: Jacutingaite family

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Transition metal dichalcogenides have been the subject of numerous studies addressing technological applications and fundamental issues. Between this class of materials, a single-layer $PtSe_2$ is a semiconductor with a trivial bandgap. In contrast, its counterpart with 25% of Se atoms substituted by Hg, Pt_2HgSe_3 (jacutingaite, a naturally occurring mineral), is a 2D topological insulator with a large bandgap. We investigate the energetic stability and the topological transition in $Pt(Hg_xSe_{1-x})_2$ as a function of alloy concentration and the distribution of Hg atoms embedded in the $PtSe_2$ host. Our findings reveal the dependence of the topological phase on the alloy concentration and robustness regarding the distribution of Hg ordered and random configuration. And also show that vacancies randomly distributed induce a quantum transition trivial to topological in doped materials. Finally, we discuss a fundamental issue is whether a topological insulator protected by time-reversal is robust enough under a transformation to an amorphous state. The crucial role of translational symmetries in building the theory of topological insulators raises the question: to what extent is translational symmetry necessary for a topological state to retain its properties?