Jacutingaite, a recently discovered Brazilian naturally occurring mineral [1, 2], has shown to be the first experimental realization of the Kane-Mele topological model [3]. In this talk we will shown that the class of materials M2NX3 (M = Ni, Pt, Pd; N = Zn, Cd, Hg; and X = S, Se, Te), share jacutingaite’s key features, i.e., high stability of its transition metal dichalcogenide like structure (Fig. 1), and topological phase. By employing first-principles calculations we extensively characterize the energetic stability of this class while showing a common occurrence of the Kane-Mele topological phase. Here we found Pt-based materials surpassing jacutingaite’s impressive topological gap (Fig. 2) and lower exfoliation barrier while retaining its stability.

References


Figures

Figure 1: Jacutingaite’s class structure in relation to the transition metal dichalcogenide.

Figure 2: Topological gap for the class of M2NX3 compounds.