Jacutingaite-family: a class of 2D topological materials

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Jacutingate, 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 wil 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

[1] A. R. Cabral, H. F. Galbiatti, R. Kwitko-Ribeiro, and B. Lehmann. Terra Nova 20, 32–37 (2008).
[2] Anna Vymazalová, Frantisek Laufek, Milan Drábek, Alexandre R. Cabral, Jakub Haloda, Tamara Sidorinová, Bernd Lehmann, Henry F. Galbiatti, and Jan Drahokoupil. The Canadian Mineralogist 50, 431–440 (2012).
[3] Antimo Marrazzo, Marco Gibertini, Davide Campi, Nicolas Mounet, and Nicola Marzari. Phys. Rev. Lett. 120, 117701 (2018)

Figures

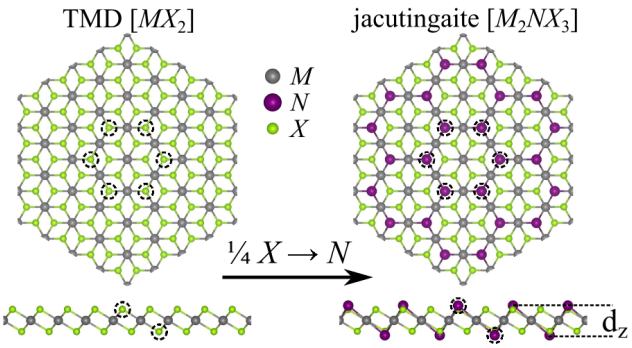

Figure 1: Jacutingaite's class structure in relation to the transition metal dichalcogenide.

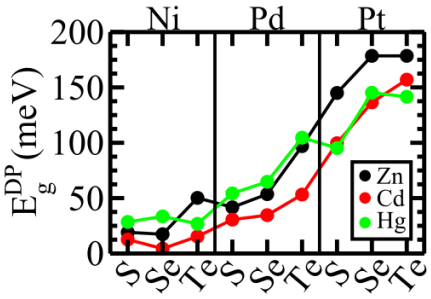

Figure 2: Topological gap for the class of M2NX3 compounds.