Polymorphic Structural Phase Transformations in 2D Materials

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Abstract

Two-dimensional (2D) materials and their associated compositional polytypes, which are materials with identical chemical compositions that decorate different crystal structures, offer unique properties with potential uses in various emerging and hypothesized technological devices. Structural phase transformations provide a means for controlling the properties of single-layer 2D materials in a reversible manner through various methods such as post-synthesis modification using strain engineering or strong light-matter interactions. Exploring the polytype phase space can aid in identifying new potential candidates for structural phase transitions. Here, we utilized the C2DB [1] to identify the feasibility of structural phase transformations for 1,555 dynamically stable compositional polytypes. Out of these polytypes, we focus on 200 2D material compositions that possess an E_{hull} < 200 meV/atom and have more than one compositional polytype, which were analyzed to assess the feasibility of each composition's thermodynamic viability for polymorphic structural phase transformation. Finally, we highlight experimentally synthesized 2D compositions.

References

[1] S. Haastrup, et. al. 2D Materials, 5 (2018) 042002.

Figures

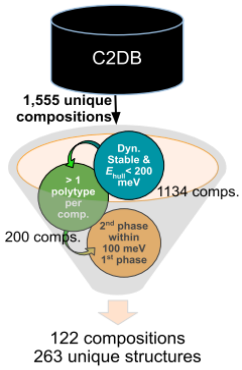

Figure 1: Selection criteria for filtering materials from the C2DB.

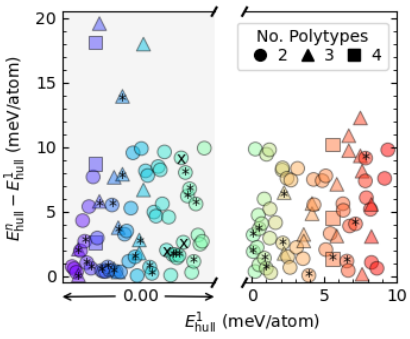

Figure 2: The relationship between the most stable primary polytype and higher energy polytypes for a given composition. The y-axis represents the difference between the higher energy and primary polytypes' E_{hull}. The x-axis indicates the E_{hull} of the primary phase. Each unique composition with E_{hull} = 0.0 is shifted horizontally to avoid overlapping data points. Marker color denotes the chemical composition, the * and x indicate 2D materials with a corresponding bulk parent structure in the ICSD/COD or has been synthesized in monolayer form, respectively, while marker shape indicates the total number of polytypes for each composition.