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Computational Discovery of a Novel Semiconductor: A Vacancy-Ordered $Fe_{1.5}TiSb$ Heusler Phase VINAY ISHWAR HEGDE, Northwestern University, NARIMAN NAGHIBOLASHRAFI, SAHAR KESHAVARZ, KAMARAM MUNIRA, WILLIAM BUTLER , PATRICK LECLAIR, The University of Alabama, CHRIS WOLVERTON, Northwestern University — Many full- and half-Heusler phase compounds are half-metallic ferromagnets, and are attractive for spintronic applications due to their relatively high Curie temperatures. However, while it is known that defects such as vacancies (on the X site of an X_2YZ Heusler phase) can lead to a loss of half-metallic character, their effect on the stability and order of these compounds has not been adequately explored. To address this shortcoming, we perform a binary cluster expansion (CE) of Fe and vacancies on the Fe sublattice of the $Fe_xVac_{2-x}TiSb$ Heusler compound. From our CE, we computationally predict the stability of a novel semiconductor phase with an interesting new structure type: $R3m$ spacegroup with composition $Fe_{1.5}TiSb$, i.e., between the full- and half-Heusler compositions. By comparing the electronic structure of all the competing structures at $x = 1.5$, we find that the gap opened in the minority-spin channel due to vacancies strongly correlates with the stability of the structure. We study the effect of vacancies on the structural order in $Fe_{1.5}TiSb$ by generating special quasi-random structures (SQSs) as approximations to the true disordered state, and find that the material undergoes an order-disorder transition at elevated temperatures of $\sim$1450 K.

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