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Computational design of new A2BX4 materials[1]

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The A2BX4 family of ternary compounds represents an important class of materials. Members of this group, in addition to being among the earth most abundant materials, also span a significant range of physical properties including ferromagnetism, coexistence of transparency and p-type conductivity, ferroelectricity, etc. Today we know for about 800 A2BX4 compounds that have been characterized experimentally. This is only a portion of nearly 5000 A2BX4 combinations that could be constructed throughout the periodic table. In this talk I will present a systematic theoretical approach, based on ab initio calculations, for predicting new A2BX4 compounds. For a given new A2BX4 combination we find the candidate crystal structures from the classification of the existing A2BX4 in terms of the atomic orbital radii of the constituent A and B atoms (Zhang and Zunger, Adv. Funct. Mat. 20, 1944, 2010). This step is followed by the set of high-throughput ab initio calculations which are used to sort out the ground-state structure and compute the corresponding heat of formation. The stability of a given A2BX4 with respect to decomposition into competing phases is then tested against all possible combinations of known compounds involving the same elements. This is done by comparing the heat of formation of the new ternary and the heats of formation of the competing (existing) binary and ternary compounds. I will also discuss the algorithms for searching the chemical space of ternary compounds in order to find the materials with target properties.

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