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Evolutionary Structure Prediction of Stoichiometric Compounds[1]

QIANG ZHU, ARTEM OGANOV, Department of Geosciences, SUNY Stony Brook, NY, 11794 — In general, for a given ionic compound A_mB_n at ambient pressure condition, its stoichiometry reflects the valence state ratio between per chemical specie (i.e., the charges for each anion and cation). However, compounds under high pressure exhibit significantly behavior, compared to those analogs at ambient condition. Here we developed a method to solve the crystal structure prediction problem based on the evolutionary algorithms, which can predict both the stable compounds and their crystal structures at arbitrary P,T-conditions, given just the set of chemical elements. By applying this method to a wide range of binary ionic systems (Na-Cl, Mg-O, Xe-O, Cs-F, etc), we discovered a lot of compounds with brand new stoichimetries which can become thermodynamically stable. Further electronic structure analysis on these novel compounds indicates that several factors can contribute to this extraordinary phenomenon: (1) polyatomic anions; (2) free electron localization; (3) emergence of new valence states; (4) metallization. In particular, part of the results have been confirmed by experiment, which warrants that this approach can play a crucial role in new materials design under extreme pressure conditions.

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