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Ab-Initio Prediction of Phase Diagrams Using a Genetic Algorithm WILL TIPTON, Cornell University, RICHARD HENNIG — The computational design and prediction of materials' properties is a goal on which much progress has been made. However, it is generally necessary to first determine a material's crystal structure, and this remains a difficult problem. Previously, genetic algorithms have been successful in searching for stable crystal structures at particular compositions. However, when approaching a new material system, it is often unknown at which compositions stable structures might form. In order to search all of composition space simultaneously, Trimarchi and Zunger have recently suggested a modification to the traditional GA approach. In this method candidate structures are evaluated according to their formation energies with repect to structure found previously. We have implemented this technique in our genetic algorithm code and are investigating the practical details of its use. We have predicted previously-unknown phases in the Li-Be and elemental Eu systems under high pressure.

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