The first principle prediction of crystal structure by combining knowledge methods with first principles energy methods.

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The prediction of structure is a key problem in computational materials science that forms the platform on which rational materials design can be performed. For many materials chemistries standard DFT approaches are highly accurate in selecting the true ground state of a system form a small set of candidate structures, though notable exceptions exist. *Finding* ground states by traditional optimization methods on quantum mechanical energy models is difficult due to the complexity and high dimensionality of the coordinate space. An unusual, but efficient solution to this problem can be obtained by merging ideas from heuristic and ab initio methods: In the same way that scientist build empirical rules by observation of experimental trends, we have developed machine learning approaches that extract knowledge from a large set of experimental information and a database of over 15,000 first principles computations, and used these to rapidly direct accurate quantum mechanical techniques to the lowest enery crystal structure of a material. *Knowledge* is captured in a Bayesian probability network that relates the probability to find particular crystal structure at a given composition to structure and energy information at other compositions. We show that this approach is highly efficient in finding the ground states of binary metallic alloys and can be easily generalized to more complex systems