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Crystal structure prediction using evolutionary algorithms: how to predict large and complex sys-

tems

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Evolutionary crystal structure prediction proved to be a powerful approach in discovering new materials. Algorithm USPEX allows one to predict the most stable crystal structure for a given compound without requiring any experimental input. However, certain limitations are encountered for systems with a large number of degrees of freedom and complex energy landscapes. We explore the nature of these limitations and address them with a number of newly developed tools. For large systems a major problem is the lack of diversity. It is countered with modified variation operators that favor atoms with higher local order and a special initialization procedure for the first generation. For complex energy landscapes, the key problem is the possible existence of several energy funnels. To address this problem, we develop an algorithm incorporating the ideas of abstract “distance” between structures using the so called “fingerprint function.” We will compare the efficiency of the old and new algorithm USPEX for different systems and show that the range of application for algorithm is increased. Some systems, where old algorithm couldn’t find a solution are now solvable with the new algorithm. And the speed of finding the solutions for systems with the complicated energy landscape is substantially increased.