

Abstract Submitted
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USPEX - Predicting crystal structures of new phases COLIN W. GLASS, ARTEM R. OGANOV, Lab. of Crystallography, ETH Zuerich — We have developed an very efficient and reliable method for crystal structure prediction [1], merging an evolutionary algorithm, based on local optimization and spatial heredity, with *ab initio* total-energy calculations. This method allows one to predict the most stable crystal structure and a large number of robust metastable structures for a given compound at any $P-T$ condition, without requiring experimental input. The success rate is extremely high – USPEX succeeded in all of the 25 tests performed so far, including ionic, covalent, metallic, and molecular structures with up to 20 atoms per unit cell. Using this methodology we have succeeded in predicting hitherto unknown structures [2]. Implementation of the algorithm, several applications and physical reasons for its success will be discussed. [1] Glass C.W, Oganov A.R., Hansen N. (2005). USPEX: a universal structure prediction algorithm. *In prep.* [2] Oganov A.R., Glass C.W., Ono S. (2005). High-pressure phases of CaCO_3 : crystal structure prediction and experiment. *Earth Planet. Sci. Lett, in.press.*

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