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Computational Materials design by Evolutionary Structure Prediction

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Crystal structure prediction (CSP) has been viewed as a major challenge in condensed matter science for a long time. Until recently, we developed a USPEX method based on evolutionary algorithms, and it proved to be a powerful tool enabling accurate and reliable prediction of structures from the beginning. How does it work - and why? In this lecture, I will summarize the principles, recent developments, and some applications of the USPEX code. 1) Optimizing chemical compositional space for compounds and co-crystals. A scheme is proposed to allow the automatic search for all the stable compounds with variation of chemical compositions. This function can be applied to study binary/ternary systems composed of both atomic/molecular blocks (Na-Cl, Mg-O, CaCl2-H2O, etc) [1]. 2) Predicting structures containing complex inorganic/organic molecular motifs. We designed a constrained evolutionary algorithm [2]. The key feature of this new approach is that each motif is treated as a building block which significantly reduces the search space. This method has been applied to a wide range of systems including inorganic complex, small molecular crystals, pharmaceuticals and even polymers crystals. 3) Predicting low dimensional system is different from predicting the bulk crystals. Surface brings another independent thermodynamic parameter, chemical potential. Since the stability of surface configuration depends on the chemical potential, the established phase diagram for multi-component system is quite different from that of bulk crystals [3].

[1] *W. Zhang, A. R. Oganov, A. F. Goncharov, Q. Zhu, et al, Science, 2013, 342, 1502-1505,* ***[2]*** *Q. Zhu, A. R. Oganov, C. W. Glass, H. T. Stokes, Acta Cryst. B, 2012, 68, 215-226,* ***[3]*** *Q. Zhu, L. Li, A. R. Oganov, P. B. Allen, Phys. Rev. B, 2013, 87, 95317*

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