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Taking Materials Design Into The Space Of Polymorphs: Structure Predictions And Realizability[1]

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The phenomenon of polymorphism exemplifies the significance of structural degrees of freedom in determining physical properties of solids. Classic case is elemental carbon with markedly different mechanical, optical and electronic properties between its graphite and diamond forms. To harness the richness of this phenomenon and extend rational materials design into the space of polymorphs, there is a need for developing approaches that are capable of exploring systematically and efficiently the potential energy surface, and (desirably) assist in experimental realization of different structures. While the former presents a common place in the field of structure predictions, less attention is given to the latter. Namely, available experimental data indicate that the energy above the ground state alone is insufficient to quantify the realizability of different structures. For example, MgO crystallizes exclusively as the rocksalt despite the predicted existence of a number of low-energy structures. Similarly, ZnO is realized in the wurtzite, zincblende and a relatively high-energy rocksalt structure, again, apparently disregarding a number of theoretically predicted low-energy structures. In this talk I will present recent attempts to tackle these issues focused on partially ionic systems. The structure prediction part is carried out by performing local DFT relaxations on a large set of random supperlattices (RSLs) with atoms distributed randomly over different planes in a way that favors cation-anion coordination. Second, application of the RSL sampling to a range of binary ionic systems such as MgO, ZnO, SnO2 and other, reveals that the frequency of occurrence of a given structure offers an estimate of the volume of configuration space occupied by the corresponding local minimum, which is shown to be connected to the realizability of different structures.

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