Modeling of Crystal Structures of Materials: Which Goals can be Achieved?

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Ability to predict structures of crystalline materials is important in many cases for practical applications. For instance, second harmonic generation by crystalline nonlinear optical materials necessarily require acentric structure of their crystals. Crystal structure is also important for high-energy materials, where molecular packing defines crystal density. Some other properties such as fluorescence, conductivity and even potency of drags are also related to their crystal structure.

We analyzed effectiveness of different force fields for crystal structure prediction for group of organic nonlinear optical, high-energy and conductive materials. It was shown that for non-planar molecules improvement of a force field could bring to a significant improvement of results. On the other hand crystal structure of planar molecules is difficult to predict, and in this case some new approaches for instance implementation of "stacking forces" should be introduced.

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