

Abstract Submitted
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Structure prediction for molecular crystals using evolutionary algorithms: methodology and applications¹ QIANG ZHU, Geosciences Department, Stony Brook University — Evolutionary crystal structure prediction proved to be a powerful approach in determining the atomic crystal structure of materials. Here, we present a specifically designed algorithm for the prediction of the structure of molecular crystals. The main feature of this new approach is that each molecule is treated as a whole body, which drastically reduces the search space and improves the efficiency, but necessitates the introduction of new variation operators described here. We illustrate the efficiency of this approach by a search for ice (H₂O) structures at zero pressure and temperature, which easily finds the structures of ice Ih and Ic, as well as the thermodynamically stable at these conditions ice XI. We successfully apply this method to finding the hitherto unknown structures of plastic phases of methane at high pressure. These structures are distinguished by an icosahedral packing of the molecules, and are likely candidate solutions for methane A and B.

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