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Computational Discovery of New Materials Under Pressure

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The pressure variable opens the door towards the synthesis of materials with unique properties, ie. superconductivity, hydrogen storage media, high-energy density and superhard materials, to name a few. Indeed, recently superconductivity has been observed below 203 K and 103 K in samples of compressed sulfur dihydride and phosphine, respectively. Under pressure elements that would not normally combine may form stable compounds, or may mix in novel proportions. As a result using our chemical intuition developed at 1 atm to theoretically predict stable phases is bound to fail. In order to enable our search for superconducting hydrogen-rich systems under pressure, we have developed XtalOpt, an open-source evolutionary algorithm for crystal structure prediction. New advances in XtalOpt that enable the prediction of unit cells with greater complexity will be described. XtalOpt has been employed to find the most stable structures of hydrides with unique stoichiometries under pressure. The electronic structure and bonding of the predicted phases has been analyzed by detailed first-principles calculations based on density functional theory. The results of our computational experiments are helping us to build chemical and physical intuition for compressed solids.