CMCC Mechanochemistry Discussions

Online Seminar Series

Theoretical Predictions of Superconducting and Superhard Materials

10:00 AM (CST)

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on the CMCC YouTube Channel:
Dr. Eva Zurek Seminar

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ABSTRACT:

The pressure variable opens the door towards the synthesis of materials with unique properties, e.g. superconductivity, hydrogen storage media, high-energy density and superhard materials. Under pressure elements that would not normally combine may form stable compounds or they may mix in novel proportions. As a result, we cannot use our chemical intuition developed at 1 atm to predict phases that become stable when compressed.

To facilitate the prediction of the crystal structures of novel materials, without any experimental information, we have developed XtalOpt, an evolutionary algorithm (EA) for crystal structure prediction. XtalOpt has been applied to predict the structures of binary and ternary hydrides with unique stoichiometries that become stable at pressures attainable in diamond anvil cells. The electronic structure and bonding of the predicted phases is analyzed by detailed first-principles calculations, as is their propensity for superconductivity. We also discuss the recent extension of XtalOpt towards the prediction of superhard materials, and the computational discovery of 43 hitherto unknown superhard carbon phases that are metastable at ambient conditions.

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