Crystal Structure Prediction Boosting Up High Pressure Discoveries

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Knowledge of crystal structures is essential if the properties of materials are to be understood and exploited. Crystal structure prediction at high pressures has recently become a topic of considerable interest,¹ and it often plays a leading role in major high-pressure discoveries.¹

CALYPSO structure prediction method² is an efficient approach based on swarm-intelligence algorithm, and it takes the advantage of swarm intelligence and structures smart learning and has been coded into CALYPSO software package (http://www.calypso.cn, free for academic use).

In this presentation, I will give a short introduction to the CALYPSO method,² and then focus on the application of CALYPSO method into exploration of high-pressure structures for several interesting systems. Exotic physics and chemistry not accessible to ambient pressure were revealed by taking examples of unexpected chemical reactions of Fe-Xe, N₂-Xe, HCl-H₂, and Hg-F₂ at high pressures with the formation of unusual stoichiometries.³ Reaction of Fe and Xe in the conditions of Earth core⁴ might provide a possible solution of “missing Xe paradox”. Emphasis will also be placed on our prediction of high-Tₖ superconductivity of H₂S⁴ and its later breakthrough experimental observation at Tₑ = 190 K.⁵

References