Computational search for new high-T_C superconductors based on lanthanoid and actinoid hydrides at moderate pressures

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Hydrogen-rich hydrides attract great attention due to recent theoretical [1] and then experimental discovery of record high-temperature superconductivity in H_3S (T_C = 203 K at 155 GPa [2]).

Here we perform a systematic evolutionary search for new phases in the Fe-H [3], Th-H [4], U-H [5] and other numerous systems under pressure [6] in order to predict new materials which are unique high-temperature superconductors.

We predict new hydride phases at various pressures using the variable-composition search as implemented in evolutionary algorithm USPEX [7-9]. Among the Fe-H system two potentially high-T_C FeH_5 and FeH_6 phases in the pressure range from 150 to 300 GPa were predicted and were found to be superconducting within Bardeen-Cooper-Schrieffer theory, with T_C values of up to 46 K. Several new thorium hydrides were predicted to be stable under pressure using evolutionary algorithm USPEX, including ThH_3, Th_3H_{10}, ThH_4, ThH_6, ThH_7 and ThH_{10}. $Fm\bar{3}m$$ThH_{10}$ was found to be the highest-temperature superconductor with T_C in the range 221-305 K at 100 GPa. Actinide hydrides show, i.e. AcH_{16} was predicted to be stable at 110 GPa with T_C of 241 K.

To continue this theoretical study, we performed an experimental synthesis of Th-H phases at high-pressures including ThH_{10}. Obtained results can be found in Ref. [10].

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