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Metal Carbides & hydrides : Structure and Superconductivity under high pressure

R. Ahuja[1]

[1]*Uppsala University, Department of Physics & Astronomy, Uppsala, Sweden*

The long-standing prediction that hydrogen can assume a metallic state under high pressure, combined with arguments put forward more recently that this state might even be superconducting up to high temperatures, continues to spur tremendous research activities toward the experimental realization of metallic hydrogen. These efforts have however so far been impeded by the enormous challenges associated with the exceedingly large required pressure. Hydrogen-dense materials allow for the rather exciting opportunity to carry out a proxy study of metallic hydrogen and associated high-temperature superconductivity at pressures within the reach of current techniques. In the present work, we have used first-principles methods in an attempt to predict the superconducting critical temperature (Tc) as a function of pressure (P) for metal-hydride systems. By comparing the obtained results, we are able to point out a general trend in the Tc-dependence on P. These gained insights presented here are likely to stimulate further theoretical & experimental studies of metallic phases of hydrogen-dense materials. CaC6 is superconducting with a critical temperature Tc of 11.5 K. Under pressure first Tc increases and then suppresses and the superconductivity of this compound is eventually destroyed at about 18 GPa. Here, we report a theoretical finding of the re-emergence of superconductivity in heavily compressed CaC6. The predicted phase III with carbon nanofoam is found to be stable at wide pressure range with a Tc up to 14.7 K at 78 GPa. For CaC2, we found that under compression, dumbbell carbon in CaC2 can be polymerized firstly into one-dimensional chain and then into ribbon and further into two-dimensional graphite sheet at higher pressure. Our results show that calcium can not only stabilize carbon sp2 hybridization at larger range of pressure but also contribute in superconducting behavior, which would further ignite experimental and theoretical interest.

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