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Superconductivity and electronic structures of Cu-doped Si and Ge clathrates[1] LIU YANG, NING CHEN, GUOHUI CAO, YANG LI, Department of Physics, University of Science and Technology Beijing, Beijing 100083, China —
We present a joint experimental and theoretical study of the superconductivity and electronic structures in type-I Cu-doped silicon clathrates and germanium clathrates. The superconducting critical temperature in $Ba_8Si_{46-x}Cu_x$ decrease with copper content increasing. No evidence in Cu-free and Cu-doped germanium clathrates demonstrates a bulk superconducting transition down to 2 K. These results are corroborated by first-principles simulations calculated from the meaning density-functional theory with plane waves and pseudopotentials. The simulation of Cu-doped clathrates has shown that Cu doping result in a decrease of electronic density of states in Fermi level, which might explain Tc decrease with Cu-doping in the BCS frame. Comparing with the electronic structure of Si clathrate, there is a less density of states on Fermi level for the Ge clathrate, which also is explained as the reason for no bulk superconductivity occurring. The theoretical study is supported by experimental investigations.

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