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Ga-doping effect on superconductivity for Ba₈Si₄₆ clathrates¹

RUIHONG ZHANG, YANG LIU, XINGQIAO MA, NING CHEN, GUOHUI CAO, YANG LI, Department of Physics, University of Science and Technology Beijing — We present a joint experimental and theoretical study of the superconductivity and electronic structures in type-I Ga-doped silicon clathrates. The superconducting critical temperature in Ba₈Si_{46-x}Ga_x is shown to decrease strongly with gallium content increasing. These results are corroborated by first-principles simulations calculated from the density-functional theory with plane waves and pseudopotentials. The simulations show that Ga doping results in a large decrease of electronic density of states in Fermi level, which can explain the superconducting critical temperature decrease with Ga-doping in the BCS theoretical frame.

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