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Pressure-induced superconductivity of solid argon and krypton from first-principles

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Searching for the superconductivity in elemental solids is of fundamental scientific interest. Electrical resistance measurements at high-pressure and low-temperature have clarified that 53 elements show the superconductivity, of which 23 are induced by pressurization [1]. However, in noble gases, insulating states exist over wide pressure range owing to closed-shell valence electron configurations, and no superconductivity has been observed experimentally.

In the present study, we focus on the superconductivity of solid argon (Ar) and krypton (Kr). Both elements take the face-centered cubic (fcc) structure at ambient pressure, which is experimentally observed to be stable up to at least 70 GPa. First-principles calculations predict the structural phase transition into the hexagonal close-packed (hcp) structure at 220 GPa for Ar and 130 GPa for Kr, in which electronic band gap closure occurs at 514 GPa for Ar and 310 GPa for Kr [2].

We explored crystal structures and the superconductivity of Ar and Kr using first-principles calculations based on the density functional theory. For Ar, our calculations predict that the double hexagonal close-packed (dhcp) structure emerges as the most stable structure in pressure range from 420 to 690 GPa, where an insulator-to-metal transition occurs at around 590 GPa [3] The crystal structure transforms into hcp at 690 GPa and into fcc at 2300 GPa. The superconducting critical temperature (T_c) is gradually increased with the successive phase transitions, dhcp → hcp → fcc, and reaches the maximum value of 12 K at 2600 GPa in the fcc phase [3]. We found that the increase of the superconductivity is caused by the increase of the Fermi surface nesting. On the other hand, Kr shows no structural phase transition from hcp and no enhancement of the superconductivity ($T_c \leq 2$ mK) up to at least 2600 GPa. These results suggest that Ar is expected to be the superconductor with the highest T_c of noble gases.

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