Highlights

RESEARCH AREA 1 - Superconductors and Innovative materials for Energy and Environment - 2024

Charge transfer in alkaline-earth metal graphite intercalation compounds

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Graphite is a common material formed by stacked graphene layers, exhibiting remarkable properties, especially when metal atoms are intercalated between graphene layers. In this study, we investigated how alkaline-earth metals as calcium, strontium, and barium enter the graphite structure to form compounds that display superconductivity. A key focus of our work is the crucial role of electric charge transferred from these metals to the graphene layers, a process that strongly influences the electronic properties and ultimately the superconducting performance of these intercalated materials.
Using high-purity bulk samples, we combined X-ray diffraction, Raman spectroscopy, and advanced DFT simulations to track how charge transfer evolves across BaC_6, SrC_6, and CaC_6. We uncovered a clear pattern: smaller metal atoms bring graphene layers closer together and transfer more charge, with calcium donating the most.
This added charge stretches carbon–carbon bonds and modifies vibrational modes, effects observed experimentally and reproduced theoretically. The calculations also show that charge accumulates differently depending on the metal species, helping explain why CaC_6 achieves the highest superconducting transition temperature.
Altogether, we provide a coherent picture of how intercalated metals reshape graphite's structural, vibrational, and electronic landscape, advancing our understanding of superconductivity in layered carbon materials.

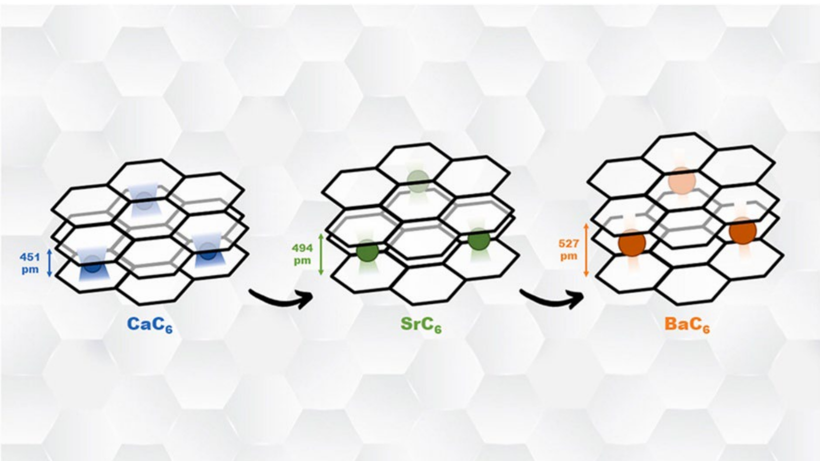

Fig. 1. A sketch of the alkaline-earth metals intercalation process in the graphite layer showing that the smaller metal atoms bring graphene layers closer, resulting in an increase of the charge transfer.