

Superconductivity at 28 K in Sodium Graphite Intercalation Compound under High Pressure

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The discovery of 15.1 K superconductivity in first-stage CaC_6 reignited interest in searching for high-temperature superconductors in graphite intercalation compounds (GICs). However, despite nearly two decades of intensive research, progress in exploring high-temperature superconductivity in GIC materials has remained stagnant. Currently, research on the superconductivity of GICs mainly focuses on first-stage GICs, while the superconductivity of high-stage GICs has been largely overlooked. Here, we report an experimental discovery of superconductivity with maximum critical temperature (T_c) of approximately 28 K in sodium carbide at about 14 GPa evidenced by a sharp drop of resistance and a characteristic decrease of T_c under magnetic fields up to 6 T. The upper critical field $\mu_0 H_{c2}(0)$ was estimated to be 8.8 T based on fitting with the Ginzburg-Landau superconducting model while the coherent length is approximately 61.2 Å. X-ray diffraction measurements combined with crystal structure predictions identified the superconducting candidate material as the second-stage GIC NaC_8 , in which sodium atoms occupy the interlayer spaces between AA-stacked bilayer graphene. The current findings not only achieve the long-sought high- T_c GICs, but more importantly, open up a new avenue for exploring high-temperature superconductors in light-element compounds.

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Since the discovery of superconductivity in Hg in 1911 [1], the pursuit of new superconductors with higher transition temperatures (T_c 's) has always been a hot topic in condensed matter physics and materials science. Low dimensionality is generally considered as a necessary ingredient for high superconducting transition temperatures. As a typical two-dimensional material, graphite has attracted significant attention in superconductivity research [2]. While graphite itself is not an intrinsic superconductor, the intercalation of guest atoms or molecules between its

layers can significantly modify its electronic structure, leading to the emergence of superconductivity. The resulting graphite intercalation compounds (GICs) serve as a promising platform for exploring high-temperature superconductors.

Since the discovery of superconductivity in alkali-metal GICs (MC_8 [3,4], $M = \text{K}, \text{Rb}, \text{or Cs}$), the superconducting behavior of GICs has been a subject of great interest. Subsequently, more superconducting GICs have been discovered; however, their T_c 's generally remain low (< 6 K) [3–12]. In 2005, a significant breakthrough in GICs research was achieved with the discovery of superconductivity in CaC_6 at 11.5 K [13,14]. Even more exciting was the finding that the T_c of CaC_6 further increases under high pressure, reaching 15.1 K at 7.5 GPa [15]. This finding further stimulated interest in exploring high- T_c superconductors within GICs. However, despite nearly two decades of extensive investigations [16–18], progress in uncovering high-temperature superconductivity in GIC materials has remained elusive.

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Currently, research on the superconductivity of GICs primarily focuses on first-stage GICs, where the stage index denotes the number of carbon layers separating the periodically inserted intercalate layers [19]. As early as the 1980s, superconductivity has been observed in second-stage GICs KHgC_8 and RbHgC_8 , with T_c 's of 1.9 and 1.4 K, respectively [20–23]. Compared to their first-stage counterparts, KHgC_4 ($T_c = 0.73$ K) and RbHgC_4 ($T_c = 0.99$ K), which contain the same intercalates, their T_c 's exhibit a significant enhancement. While the underlying mechanism has yet to be definitively established, these findings have paved a new way for the exploration of high-temperature superconductors in GICs.

Previous experimental study has demonstrated the formation of low-stage Na-GICs under high pressure without heating [10], and recent theoretical research has also proposed some thermodynamically stable second-stage sodium GICs under high pressure [24]. These results show that it is feasible to synthesize second-stage GIC in sodium-carbon systems by means of high pressure. In this work, we conducted high-pressure experimental studies on the crystal structure and superconducting properties of the sodium-graphite mixture. Notably, electrical transport measurements identified a maximum T_c of ~ 28 K at about 14 GPa, nearly twice that the value observed for CaC_6 under high pressure [15]. Based on the further analysis of x-ray diffraction (XRD) measurements [25–27] and crystal structure predictions [28–30], we propose the second-stage GIC NaC_8 as a candidate superconducting phase. This structural framework provides a prototype for exploring novel multistage GIC superconductors, particularly through the substitution of sodium with elements of lower electronegativity or more valence electrons, which may enhance metal-graphite interactions and tune the electronic properties.

We have prepared nine cells designated as Cell_1 to Cell_9 (detailed information about these cells is provided in Table S1 [31]). The samples were cold-compressed at room temperature without laser-heating treatment (except Cell_4). The representative electrical resistance measurements on Cell_1 to Cell_5 as a function of temperature at high pressures are shown in Fig. 1(a), which exhibit superconducting transitions as evidenced by the sharp drop of the resistance at 9.2, 18.8, 21.1, 21.4, and 24.8 K at about 10.5, 22.2, 17.0, 16.0, and 18.0 GPa, respectively. The T_c values are determined from the intersection of the linear extrapolations of the normal state and the transition-region resistance-temperature curves near the superconducting transition point as shown in Fig. 1(a). The observations of zero resistance exclude the possibility that the abrupt drop of resistance at low temperatures arises from structural transitions. To determine the highest value of T_c , we study its dependence on pressure, as shown in Fig. 1(b) and Figs. S1–S6 [31]. When the pressure is increased to 8.7 GPa, superconductivity emerges in the sample

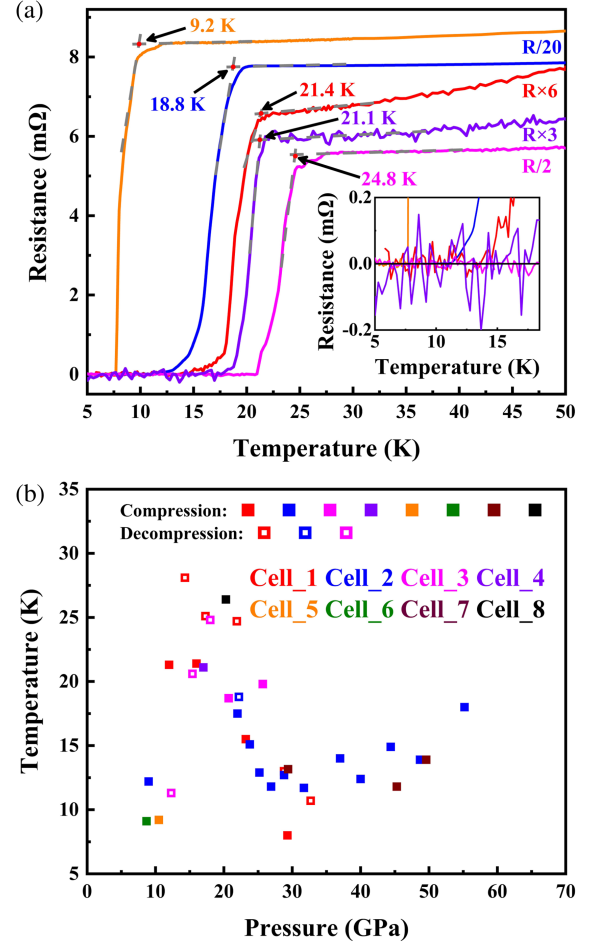


FIG. 1. (a) Superconducting transitions determined by electrical resistivity measurements in cells. The resistance data with near zero values are highlighted on a smaller scale in the right-bottom inset. The blue and magenta curves represent the data from the samples of Cell_2 at 22.2 GPa and Cell_3 at 18.0 GPa during decompression, respectively. Similarly, the red, purple and yellow curves correspond to the data from the samples of Cell_1 at 16 GPa, Cell_4 at 17.0 GPa, and Cell_5 at 10.5 GPa during compression, respectively. (b) The dependence of the critical temperature T_c on pressure. The results from different experiments are marked in different colors. The solid and open symbols represent the data obtained on compression and decompression, respectively.

(Fig. S5(b) [31]). As the pressure increases, the T_c begins to increase, reaching the highest value of 28.1 K at 14.3 GPa (Fig. S1 [31]) and then decreasing until the pressure rises to about 32 GPa. Upon further compression, the T_c increases again until the pressure reaches 55 GPa. At higher pressures, the resistance-temperature curves exhibit poorer quality (Figs. S2 and S6 [31]), potentially indicating decomposition or a phase transition of the superconducting phase. In addition, we carried out laser heating on mixed Na-graphite samples (Fig. S4 [31]) and conducted experiments using fullerene (multiwalled nanotube) as the carbon

source (Fig. S7 [31]); however, neither approach succeeded in producing a high-temperature superconducting phase.

To confirm the superconducting nature of the transitions, we further study its dependence on external magnetic fields. An applied external field could break the Cooper pairs due to the Pauli paramagnetic effect of electron spin polarization and the diamagnetic effect of the orbital motion, thus reducing the value of T_c . As shown in Fig. 2(a), the resistance drop gradually shifts to lower temperatures as the applied magnetic field increases from 0 to 6 T at 25.7 GPa, indicating a clear suppression on T_c from 19.8 to 8.5 K. Notably, when the magnetic field exceeds 6 T, the data exhibits a poor signal-to-noise ratio, making it impossible to measure the upper critical magnetic field $\mu_0 H_{c2}(0)$ directly. The upper critical field $\mu_0 H_{c2}(T)$ as a function of temperature, which is defined as 90% of the resistance, is shown in Fig. 2(b). The extrapolated value of the critical field $\mu_0 H_{c2}(0)$ is 8.8 T fitted by the Ginzburg-Landau (GL) model. The magnitude of the estimated coherence lengths of 61.2 Å is well below the typical

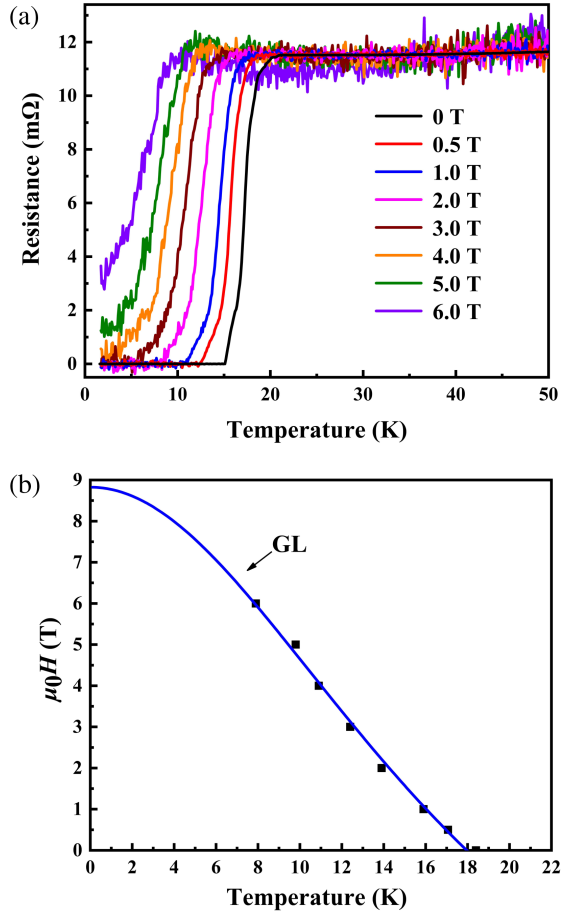


FIG. 2. (a) Temperature dependence of the electrical resistance under applied magnetic fields at 25.7 GPa. (b) Critical field $\mu_0 H$ as a function of temperature, determined using the criterion of 90% of the resistance in the metallic state at 25.7 GPa and fitted with GL model.

value (hundreds of angstroms) for type-I superconductors, indicating the sample is a type-II superconductor.

The critical current density (J_c) is another key parameter for superconductors. To estimate J_c , we first investigated the critical currents (I_c) for the sample in Cell_7 within the current range of 10^{-5} to 10^{-1} A under different magnetic fields at 20.2 GPa. Figure 3(a) displays the voltage-current curves of the synthesized samples at different temperatures under zero magnetic field. As the current increases, the superconducting state is gradually destroyed, which provides another evidence for the superconducting transition. Figure 3(b) shows the critical current fitting curve at different magnetic fields (including zero magnetic fields) utilizing a conservative GL model [48] $I_c = I_c(0) \times (1 - T/T_c)^{3/2}$. By extrapolating to $T = 0$ K, the critical current $I_c(0)$ is determined to be 0.0608 A. The estimate of J_c is based on the fact that the sample will not exceed the chamber size (70 μm) and the thickness is less

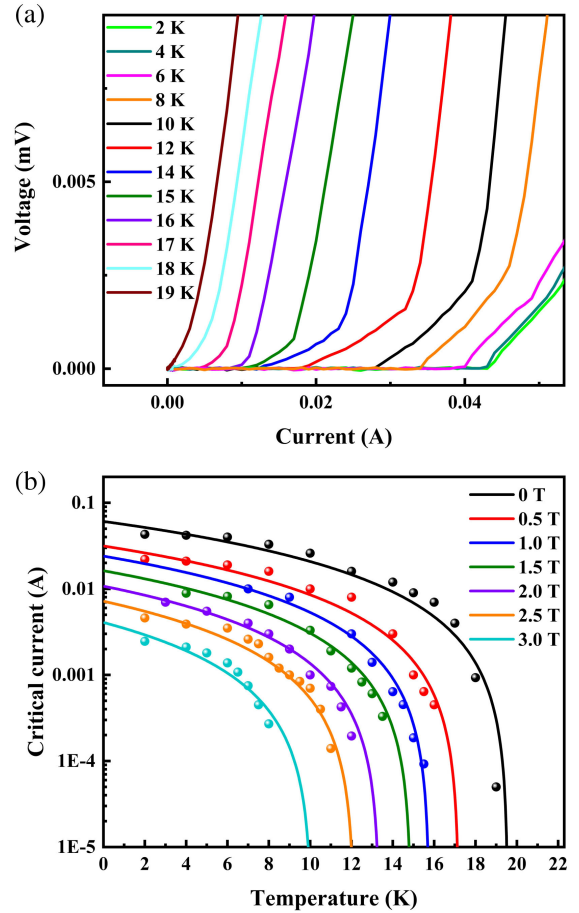


FIG. 3. The critical current measurements of NaC₈ at 20.2 GPa. (a) Representative current-voltage characteristics observed under zero magnetic fields. I_c is determined at the points where the voltage deviates from zero in the curves. (b) Extrapolation of the temperature dependence of critical current at different magnetic fields. The dots are the experimental data, and the curves are plotted by fitting the formula $I_c = I_c(0) \times (1 - T/T_c)^{3/2}$.

than the thickness of the initial sample (16 μm), and the $J_c(0)$ could potentially exceed 54.3 A/mm².

To determine the crystal structure of the superconducting products with the highest T_c , XRD measurements were performed on Cell_1 at 14 GPa. The diffraction patterns did not match the precursors (Fig. S8 [31]) or any previously reported Na-C compounds [24,47,49,50]. Using CALYPSO crystal structure prediction software, we have identified a dynamically stable *Cmcm*-NaC₈ phase (Fig. S9 [31]), whose formation enthalpy also lies on the convex hull relative to the Na-graphite system (Fig. S10 [31]). The simulated diffraction pattern is highly consistent with the experimental results (Fig. 4), suggesting that this structure is a promising candidate for the superconducting phase. The refined lattice parameters (Table S2 [31]) are $a = 14.057(2)$ Å, $b = 5.187(2)$ Å, and $c = 4.291(0)$ Å ($V = 312.90(9)$ Å³). The atomic coordinate information

of NaC₈ has been shown in Table S3 [31]. Interestingly, NaC₈ is a second-stage GIC, in which sodium atoms occupy the interlayer spaces between AA-stacked bilayer graphene in its structure. These sodium atoms are positioned off-center from the honeycomb structure, forming zigzag chains arranged in an ABAB stacking pattern along the c axis. The characteristics of this structure are consistent with previous findings, which indicate that low-stage Na-GICs can only be obtained under high-pressure conditions [10] and that AA stacking is less stable than AB bilayer stacking, with intercalation capable of inducing a spontaneous transition from AB stacking to AA stacking [51]. Notably, there are two non-GIC structures Na₂C₃ [49] and NaC₃ [50] lie on the convex hull (Fig. S10 [31]). In these two stable non-GIC structures, the carbon atoms have shifted from graphite's original hexagonal rings layers to either pentagonal rings chainlike structures (Na₂C₃) or alternating pentagonal-octagonal motifs layers (NaC₃), as shown in Fig. S10(b) [31]. Since the transformation from graphite's hexagonal rings structure to either of these phases involves a substantial energy barrier, the synthesis of NaC₈ from graphite under cold compression conditions becomes highly feasible.

The electronic structure simulation for primitive cell (Fig. S11 [31]) reveals the metallic nature and the density of states at the Fermi level are dominated by π orbital of graphene. In NaC₈, the states at the Fermi level mainly originate from π - π interaction between graphene layers, particularly within bilayer regions that are not intercalated with Na atoms [Figs. S12(a), (b) [31]]. By contrast, such π - π contributions are absent at the Fermi level in the first-stage GICs like NaC₄ [Figs. S12(c), (d) [31]]. This distinction in electronic structure indicates that the second-stage configuration of NaC₈ may enable a unique superconducting mechanism.

Previous studies have demonstrated that the T_c of GIC superconductors is closely related to the distance d between the intercalant atom and the graphite plane, where smaller d values tend to enhance T_c [19]. This effect arises because as intercalant electrons move closer to the graphite plane, the deformation potential of the intercalant and the out-of-plane vibrational modes of carbon atoms increases [52–54]. This trend has been well-established through superconducting studies of BaC₆ ($d = 2.62$ Å, $T_c = 0.065$ K [18]), SrC₆ ($d = 2.47$ Å, $T_c = 1.65$ K [16]), and CaC₆ ($d = 2.26$ Å, $T_c = 11.5$ K [13,14]). Furthermore, it has been reinforced by findings in CaC₆ ($d = 2.15$ Å [53], $T_c = 15.1$ K [15]) under high pressure. In NaC₈, the d value is 2.12 Å, even smaller than that of CaC₆ at high pressure, which may contribute to its enhanced superconductivity. Notably, within the pressure range of approximately 14–32 GPa, the T_c increases as the pressure decreases, presenting a trend contrary to the aforementioned conclusion. This phenomenon may be attributed to the structural transformation, as illustrated in Fig. S13 [31].

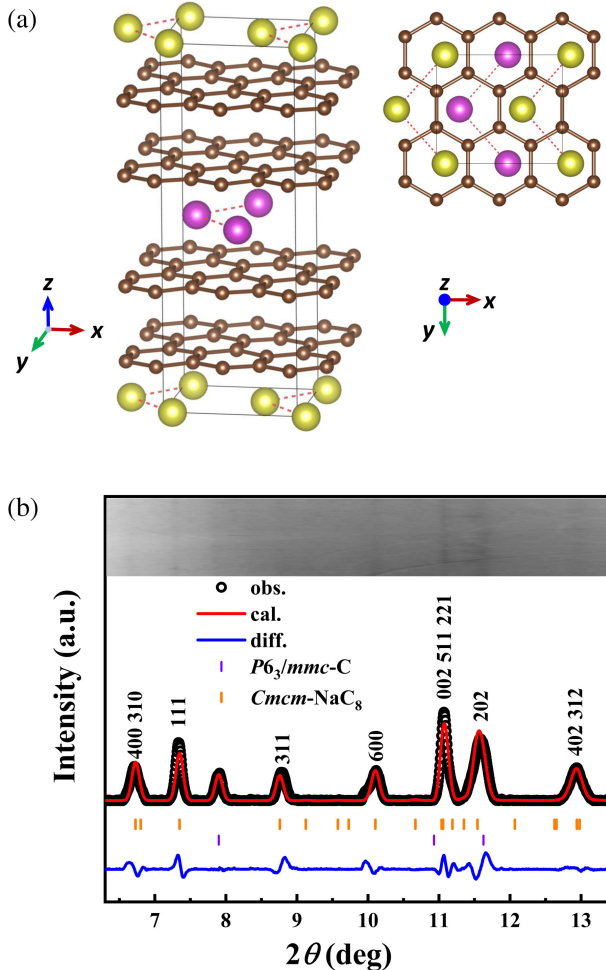


FIG. 4. (a) The crystal structure of predicted *Cmcm*-NaC₈. The yellow and pink spheres represent Na atoms, while the brown spheres represent C atoms. (b) Synchrotron x-ray diffraction pattern of the sodium-carbon compound from Cell_1 at 14 GPa and the Rietveld refinement of *Cmcm*-NaC₈.

Theoretical studies on the many-body instabilities of AA-stacking bilayer graphene have suggested that electron doping can induce a superconducting transition. This aligns with our observation of superconductivity in second-stage NaC₈, where each Na atom transfers 0.75 e^- to the graphene layers as shown in Bader charge analysis (Table S4 [31]). The two Dirac cones at -1.3 eV below the Fermi level in band structure (Fig. S11 [31]) further provide direct evidence for the electron doping effect of Na on graphene. However, accurately calculating the critical temperature in these high-stage GICs remains a challenge [55]. Especially under high-pressure conditions, the complex stress environment in the sample chamber may induce twisting between graphite layers, further complicating the calculation of the T_c . This Letter provides a foundation for studying the superconducting mechanism for electrons doping AA-stacking bilayer graphene.

In summary, we have successfully synthesized a sodium-carbide superconductor in a diamond anvil cell, exhibiting a T_c of 28 K at a pressure of ~ 14 GPa. A second-stage GIC NaC₈, in which sodium atoms occupy the interlayer spaces between AA-stacked bilayer graphene, is proposed as a promising candidate for this superconducting phase. These studies expand the prospects for developing high- T_c superconductors in GICs, substantially increasing structural diversity and offering considerable potential for discovering and exploring light-element superconductors with elevated critical temperatures.

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Data availability—The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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