Extended Abstract

Corrugated Graphene Sheets Including SeH_2 Molecules

Mohammad Amin Rastkhadiv*

Estahban Higher Education Center-Shiraz University, Estahban, Iran

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In this paper, our system under study consists of two corrugated graphene layers with SeH_2 molecules placed between them. Using the lowest-order constrained variational method, the thermodynamic and structural behavior of this system, including entropy, free energy, specific heat capacity, and the critical point, have been calculated. The results reveal a superconducting transition within a specific range of temperature and density. Therefore, the magnetic susceptibility, superconducting energy gap, and critical current density have also been evaluated. Our calculations indicate a superconducting transition temperature of about 148 K without applying external pressure and a critical current density of 10^7 A/cm². These results suggest that the proposed structure can be considered a promising candidate for superconducting applications at intermediate temperatures.

Keywords: Superconductivity; Graphene; Phase transition; SeH_2

INTRODUCTION

After the first superconductors were discovered, researchers sought materials with higher transition temperatures. A major milestone was achieving superconductivity at 250 K under roughly 100 GPa [1], though such extreme pressures limit practical use. For this reason, cuprate superconductors with T_c=133.5 K remain the most useful at ambient pressure [2]. Studies on materials with higher T_c show that they typically require very high pressures and contain large quantities of hydrogen. Hydrogen-rich compounds may exhibit strong electron-phonon coupling under compression, enabling high-temperature superconductivity, while transition metals mainly stabilize the structures [3].

Density functional theory based on Migdal-Eliashberg theory has been key in predicting T_c for clathrate hydrides, where atoms such as Y, Ca, or La sit inside hydrogen cages. Structures like CaH_6, YH_6, YH_{10}, and LaH_{10} have predicted transition temperatures between 235 and 320 K at pressures near 0.1 TPa. However, theoretical predictions often disagree with experiments due to difficulties modeling hydrogen anharmonicity [4].

Our earlier work [5] used the lowest-order constrained LOCV method to study graphene layers containing impurity molecules such as H_2S, H_3S, and CeH_9. CeH_9 displayed a second-order phase transition with T_c=186.3 K. In later work, we identified an optimal molecular arrangement and calculated the superconducting gap and critical current density.

* Corresponding Author: rastkhadiv@shirazu.ac.ir

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In the present study, we investigate two graphene layers with SeH_2 molecules, computing their free energy, electronic structure, and thermodynamic properties, and demonstrating evidence of a superconducting transition.

METHOD

We use the LOCV method to compute the thermal, electrical, and magnetic properties of the system's valence electrons. LOCV is well suited for studying critical systems because it introduces no free parameters into the energy expansion. The total energy is expressed as a cluster expansion, where higher-order terms become negligible. Since we also include spin-spin interactions, the total number of electrons is divided into spin-up and spin-down groups, and their Fermi-Dirac distributions are used to calculate the chemical potential and the spin-ordering parameter. In LOCV, the many-body fermionic wave function is written as a product of an Slater determinant and a correlation function. The system's energy is then obtained from cluster energies, where the two-body effective potential depends on correlation functions that satisfy Euler-Lagrange equations.

Entropy, magnetic susceptibility, and other thermodynamic functions are computed from standard statistical mechanical relations. For magnetic properties, an external field along the z-axis is included. The model also contains a detailed structural configuration: two corrugated graphene layers separated by distance L, with SeH_2 molecules placed between them. Determining the equilibrium atomic positions is essential, so trial coordinates are optimized by minimizing the free energy. Carbon, selenium, and hydrogen atoms are treated as ions, and valence electrons form a fluid that moves through the lattice. Finally, single-electron energies and wavefunctions are obtained by solving the Schrödinger equation for electrons interacting with carbon and dopant ions. These serve as inputs for calculating all thermodynamic properties of the system.

RESULTS AND DISCUSSION

Critical temperatures were computed for 9,900 molecular configurations, with cluster expansions truncated at the third term, and all energetic quantities expressed per particle. Free energy was minimized over structural parameters, demonstrating structural stability across temperatures and densities. Free-energy curves reveal an unstable region and two minima, indicating a first-order transition that evolves into a second-order phase transition at the critical point. Using a modified Maxwell double-tangent method, the critical temperature was found to be $T_c = 147.83$ K. This is approximately 14 K higher than the highest T_c known in cuprates at ambient pressure. Importantly, no external pressure is required; the internal fermionic pressure suffices.

The effective electron mass near the critical point lies in the range 0.16–0.36 m, showing a strong attractive interaction mediated by phonons. Removing the effective mass eliminates the transition entirely, highlighting the essential role of electron-phonon coupling. The grooved graphene structure and the hydrogen-rich SeH_2 molecules together support the required phonon spectrum.

Specific heat C_v displays critical divergence, while magnetic susceptibility χ shifts from small positive values above T_c to nearly −1 below T_c, indicating almost perfect diamagnetism (Meissner-like behavior). Energy-gap calculations $\Delta(T)$ confirm superconductivity, with the temperature dependence fitting a standard power-law model. The reduced gap ratio $\alpha = 2\Delta_0 / (k_B T_c) \approx 6.68$ greatly exceeds the BCS weak-coupling value 3.5, placing the system firmly in the strong-coupling superconducting regime. The calculated critical current density J_c reaches approximately 10^7 A/cm², comparable to high-performance cuprate-based coated conductors. The combination of high T_c, strong coupling, and high J_c makes this graphene-SeH_2 bilayer system a promising candidate for superconducting wire and device applications.

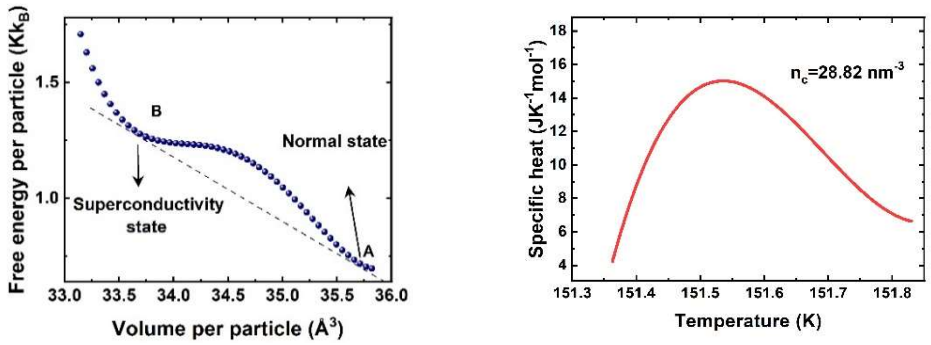


Figure 1. Left: Free-energy diagram of the electron fluid, per electron, as a function of the inverse density at temperature T=146 K. Right: Plot of the constant-volume specific heat for the conduction electrons at the critical density and near the critical temperature.

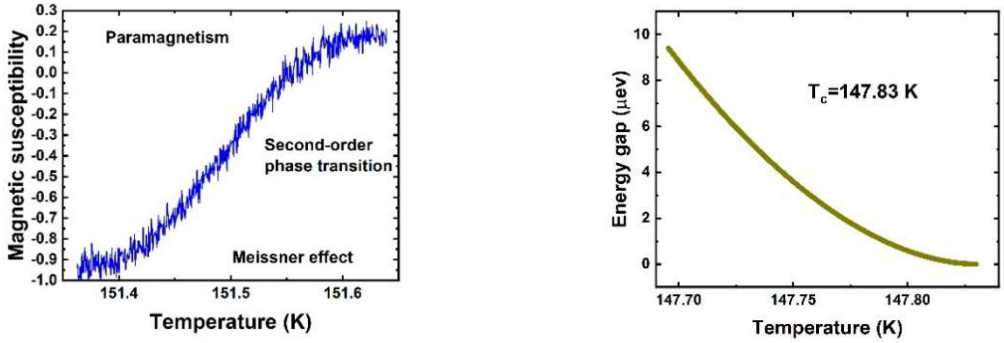


Figure 2. Left: Magnetic susceptibility of conduction electrons in the vicinity of the critical temperature. The second-order phase transition and the Meissner effect are clearly visible. Right: Superconducting energy gap of the system as a function of temperature.

CONCLUSION

In this study, we investigate a superconducting phase transition in valence electrons of a two-layer graphene system doped with SeH_2 molecules. We have examined 9900 distinct SeH_2 distributions and calculated their critical temperatures. The highest value, T_c=147.83 K, exceeding the critical temperature of $HgBa_2Ca_2Cu_3O_{x+\delta}$ by about 14 K. No external pressure was applied to the graphene layers; the effective critical pressure arises from interactions between valence electrons, their environment, and the overall fermionic wave function. Our results show that neglecting spatial variation and effective mass eliminate the superconducting transition, highlighting the essential role of phonon-phonon and phonon-electron interactions in Cooper-pair formation.

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