Title: Investigation on the spectroscopic characteristics and electrical transport of boron doped graphene system

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Abstract

Condensed Matter Physics (CMP) displays captivating diversity through the interplay of energy and length scales. CMP's collaboration among theorists, experimentalists, and engineers has revolutionized finding exotic substances. Graphene, a single layer of carbon atoms in a hexagonal lattice, has drawn immense materials science attention with its exceptional properties — electrical/thermal conductivity, mechanical strength, and transparency — enabling diverse applications. One of the key aspects that make graphene versatile is its property tunability through a process called doping. Doping allows for precise adjustments of graphene's characteristics, opening up avenues for customizing its properties to suit specific needs in many applications. This thesis is focused on delving into the spectroscopic investigation of electronic and vibrational properties within doped graphene. This work also deals with the understanding the carrier transport properties in this modified two-dimensional system.

Introducing light elements to specific sites within the graphene lattice holds exciting potential, including adjustable bandgaps, heightened electron-phonon interaction, and unconventional transport characteristics. relevant to superconductivity (SC), ferromagnetism, and catalysis. However, this strategy can inadvertently introduce more defects and strain-related consequences as residual effects, leaving room for interpretation. Boron doping, the deliberate introduction of boron atoms into the graphene lattice, has emerged as a powerful strategy to modify and enhance graphene's properties. In this dissertation, various doping methods, including chemical vapor deposition, thermal treatment, and chemical synthesis, highlighting their advantages and limitations have been discussed. Boron-doped graphene exhibits fascinating properties, such as increased carrier concentration, improved catalytic activity, and enhanced stability under harsh conditions. These attributes make it highly promising for applications in electronic devices, energy storage, and catalysis. The challenges and opportunities associated with boron-doped graphene, including the need for precise control over doping levels, potential toxicity concerns, and the quest for scalable synthesis methods have been explored in this work. Moreover, it elucidates emerging trends and future prospects, emphasizing the role of boron-doped graphene

in advancing nanotechnology and materials science. Boron doping in graphene opens up exciting avenues for tailoring its properties, expanding its utility, and pushing the boundaries of what is possible in the world of two-dimensional materials.

In the initial phase of our research, a spectroscopic approach in conjunction with ab-initio results has been employed to unravel these intricacies. Through in-situ boron-doped reduced graphene oxide specimens, this work explored a range of hole doping concentrations, achieved by tuning annealing temperatures up to 1000°C. The thesis has shown, by varying the concentration and configuration (BC_3, BCO_2, BC_2O), a distinct interplay emerges, wherein the dopant competes with residual surface oxygen atoms. The study reveals a transition of preferred doping configuration from out-of-plane to in-plane (substitutional) with rising temperature. Additionally, as the doping concentration increases, the graphene lattice experiences both point defects and strain-induced effects. These factors lead to an anomalous bandgap crossover at elevated temperatures in boron-doped graphene, setting it apart from the thermally reduced counterpart. This observation bears significance for electronic and transport applications.

Moving forward in our research, the interaction between electrons and phonons in the subsequent phase has been inspected with assistance of some spectroscopic tools. While pristine graphene exhibits exceptional electrical conductivity, the induction of charge density wave (CDW) has been a challenging endeavour. CDW, periodic modulations of electron density accompanied by lattice distortions, are central in understanding novel phenomena in low-dimensional materials.

Traditionally, inducing CDW in graphene has proven elusive due to its inherent electronic structure. The direct application of in-plane perturbations or gating techniques often falls short of creating the conditions required for CDW formation. Recent research has highlighted the crucial role of out-of-plane doping, which involves introducing foreign atoms or molecules into the graphene lattice perpendicular to the carbon plane. In the literature, metal-intercalated graphene has already emerged as a promising strategy to induce symmetry-breaking phase transitions such as SC and CDW in two-dimensional layered materials. This approach capitalizes on the modified electronic and phonon structure of metal-intercalated graphene compared to its pure counterpart. By incorporating soft vibrations and accumulating charges within the interlayer region of few-layer graphene, a potent carrier-lattice interaction and extensive charge ordering can be achieved, opening avenues for unique electronic

vibrations and accumulating charges within the interlayer region of few-layer graphene, a potent carrier-lattice interaction and extensive charge ordering can be achieved, opening avenues for unique electronic phenomena. Furthermore, out-of-plane doping facilitates the emergence of a bandgap near the Fermi level, making CDW more attainable.

This thesis reviews experimental and theoretical studies that demonstrate the effectiveness of out-of-plane doping in realizing CDW in graphene. It discusses various doping techniques, such as chemical adsorption, intercalation, and substitution, and their impact on the electronic structure. The resulting CDW offer exciting possibilities for tailored electronic, thermal, and optical properties, with potential applications in advanced nanoelectronics and quantum technologies.

Overall, this abstract emphasizes the necessity of out-of-plane doping as a powerful tool for achieving charge density waves in graphene. By understanding and harnessing the role of out-of-plane dopants, researchers can unlock the full potential of graphene in the realm of emergent electronic phenomena and pave the way for next-generation graphene-based devices. In this context, boron-doped few-layered graphene stands out as a key player in realizing CDW phases at elevated temperatures (above T = 100K). The presence of out-of-plane boron groups proves instrumental in driving this transition. Ab-initio simulations unveil a distinctive CDW energy gap within the material's band structure, a finding corroborated by low-temperature electrical transport measurements. This study not only establishes a connection between the structural and vibrational characteristics of boron-doped few-layered graphene in the CDW ordering context, but also uncovers an intriguing electric field dependence on the CDW phase in this non-metallic, light-atom-doped graphene system.

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