INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Two-dimensional materials are being widely investigated for the development of futuristic electronic devices and creating new opportunities in electronic industries. Graphene having a hexagonal honeycomb planar structure of sp2-hybridized carbon atoms has shown extraordinary electronic, mechanical and thermal properties and is considered as a potential material for use in future electronic devices. Several computational methodologies using first principles methods are providing results close to the experimental observations. Complex quantum mechanical calculations are successful in computing equilibrium in interacting materials, optical spectra, energies, electronic properties, and catalytic properties of atoms, molecules and atomic/molecular systems.

This thesis mainly focuses on the research work carried out using density functional theory (DFT) based modelling to analyze electronic properties of graphene doped with 4d-transition metal atoms, interaction of niobium-doped graphene with small molecules, spin transport properties of niobium-doped AGNR, interaction of graphene with niobium and niobium compounds, and graphene-heptahelicene interface. $DMoL^3$ code is employed to investigate single and double vacancy graphene doped with 4d-transition metal atoms and calculate their binding energies, band structures, magnetic properties, the density of states (DOS), atom projected density of states (PDOS), and charge transfer.

Niobium-doped graphene is investigated for sensing small molecules viz., CO, NH_3, CH_4, SO_2, and H_2S. Adsorption energy, equilibrium adsorption distance, DOS, PDOS, Hirshfeld charge transfer, and electron localization function are calculated to understand the physisorption or chemisorption nature of adsorption. Niobium-doped AGNR is examined for NDR property as well as spin transport using local spin density approximation (LSDA) methods in Atomistix Toolkit (ATK). Spin-resolved band structure properties are observed near Fermi level. High spin filter efficiency is observed for antiparallel spin configuration of electrodes.

Further, the interaction of graphene with Nb(111), Nb(110), niobium monoxide (NbO), niobium carbide (NbC), and niobium nitride (NbN) surfaces is presented. The surfaces are geometrically optimized and binding energies, Fermi level modification and charge redistribution over the interfaces are computed using DMoL^3 code with van der Waals interaction. Finally, graphene-heptahelicene interface is geometrically optimized using CASTEP code, and optical absorption properties and band gap tuning with an applied electric field are observed.