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Analysis ofQuantumTransportforaGrapheneby the Help of GoldElectrodes

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Abstract: *Abintio quantum transport calculations based on the method of numeric localized atomic orbitals, pseudopotentials and Density Functional Theory have been performed, using SIESTA &TranSIESTA codes, for a graphene nanostructure using gold electrodes. Non equilibrium Green's Functions method have been used in conjuction with Density Functional Theory, as implemented in TranSIESTA, for calculations of transmission function, density of states and voltage-current characteristic. Transmission function and density of states show a discrete band structure which varies with applied voltage. In the voltage-current characteristic current shows non-linear fluctuating pattern with increase in voltage and lies in the pico-ampere range.*
Keywords: *Graphene, Transport properties, Density functional theory, SIESTA, TranSIESTA, Transmission Function.*
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I. INTRODUCTION

Carbonbasedmaterialssuchasgraphene(asingl hexagonalstructureofcarbonatoms)havegeneratedalotofinterestduetotheirexoticelectronicproperties [1-3].Novelcondensedmattereffectsarisingfromits uniquetwodimensional(2D)energydispersionalong withsuperiorpropertiesmakeitapromisingmaterial fornextgenerationoffaster&smallerelectronic devices.

Studyoftransportpropertiesofnanostructures iscurrentresearchinterest[4-7].Inthispaperwehave performedfirstprinciplequantumtransport calculationsforgraphenenanostructureattachedto goldelectrodesusingTranSIESTA[7,8]which calculatestransportpropertiesusingnonequilibrium Green'sfunctionapproach.Transmissionfunctions, electrondensityofstates,projecteddensityofstates andcurrent-voltagecharacteristichavebeencalculated (seeFigure1).

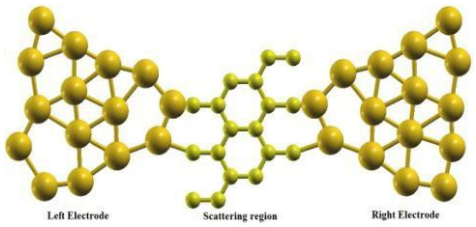


FIGURE1. Schematicviewofgraphenenano structurealongwithgoldelectrodes.Centralpartisthe scatteringregion,leftandrightpartsaregold electrodes.

II. SIMULATION DETAILS

Wehaveperformedabinitiocalculationswithinthe frameworkofDFTasimplementedinSIESTAcode [8].TroullierMartin,normconserving,relativistic pseudopotentialshavebeenusedforbothcarbonand gold.Theexchangeandcorrelationenergiesare treatedwithinthegeneralizedgradientapproximation (GGA)accordingtothePerdew,BurkeandErnzerhof (PBE)parameterization.Throughoutthegeometry optimization,numericalatomicorbitalswithsingle zetapolarization(SZP)basissetwithconfinement energyof0.01Rywereused.TheBrillouinzonewas sampledusingMonkhorst-Packschemewitha1×11×40meshforthecalculationsand250Rymesh cutoffenergywasused.Aninteractionbetween

adjacentgraphenelayersishinderedbyaspacingof20Å.Thescatteringregionconsistsofagraphenenanostructurecontaining18Catomsintheformof3x3x1supercell.Theelectronictransportproperties arestudiedbythenonequilibriumGreen'sfunction techniques,withintheKeldyshformalism[9],based ondensityfunctionaltheoryasimplementedinthe TranSIESTAmodulewithintheSIESTA.Thecurrent throughthecontactregionhasbeencalculatedusing Landauer-Buttikerformula[10]

Where$G_0=2(e^2/h)$istheunitofquantum conductanceand$T(E,V_b)$isthetransmission probabilityofelectronsincidentatanenergyE throughthedeviceunderthepotentialbiasV_b.The electrochemicalpotentialdifferencebetweentheleft andrightelectrodesis$eV_b = \mu_L - \mu_R$.

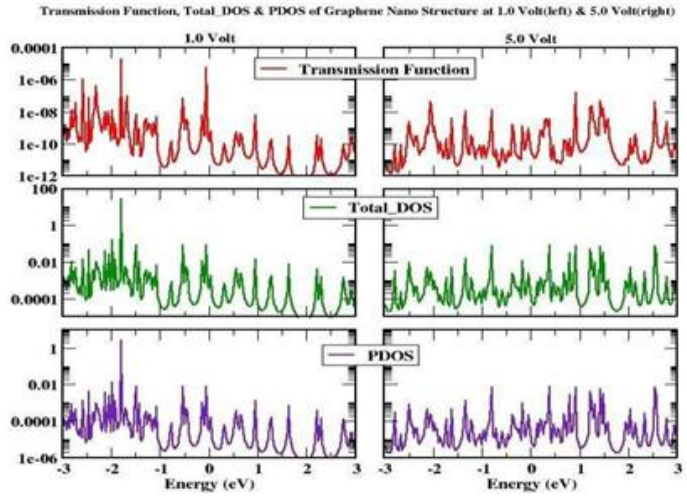
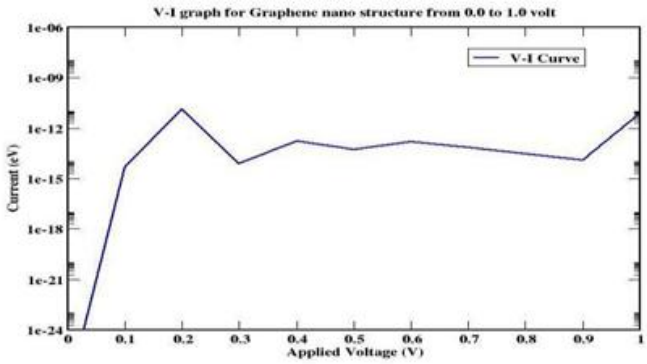
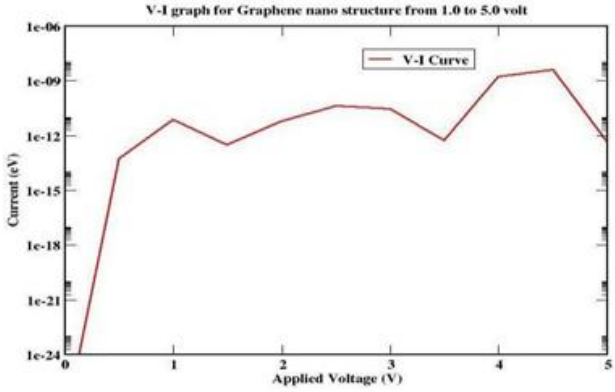


FIGURE2. Transmissionfunction,totaldensityof states(DOS)andprojecteddensityofstates(PDOS)of GrapheneNanoStructureat1.0Vand5.0V.



(a)



(b)

FIGURE3. Voltage-Current(V-I)characteristicsfor graphenenanostructure(a)forappliedvoltage0.0V to1.0Vat0.05Vsteps(b)forappliedvoltage0.0Vto5.0Vat0.25Vsteps.

III. RESULTS AND DISCUSSION

Figure2showsthetransmissionfunction,totaldensity ofstates(DOS)andprojecteddensityofstates(PDOS) ofGrapheneNanoStructureat1.0V&5.0V.

Itisclearthatthetransmissionfunction,projected densityofstatesandtotaldensityofstatesshowa discretebandstructurewhichvarieswithapplied voltage

Figure3(a&b)showstheVoltage-Current(V-I) characteristicsforgraphenenanostructure.Itis observedthatintheV-Icharacteristiccurrentshows non-linearbehaviorfluctuatingwiththechangein voltage.

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