A Numerical Study of the Interaction between 1D Carbyne Chains and ssDNA

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Degree: Ph.D., December 2016
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Background/Relevance
• Biosensors function based on the electrical and mechanical properties associated with the interaction between the sensing elements and biomolecules.
• Current applications of biosensors to sequence DNA lack the required spatial resolutions.

Innovation
• The research involves using the thinnest possible nanowire, carbyne, as a sensing element to increase the spatial resolution at the single molecule level.
• Carbyne has performed extreme mechanical performance and double the stiffness of graphene and diamond.

Key Results
• First principle simulation using density functional theory (DFT) and non-equilibrium Green’s function (NEGF)
  – Codes: Quantum ESPRESSO & wannier90
  – Carbyne chain of 16 carbon atoms and carbyne chain of 16 carbon atoms attached to two graphene sheets on both sides
    – ssDNA of one base at a time
• Molecular Dynamics simulation (MD)
  – Code: NAMD
  – Carbyne chain of 16 carbon atoms
  – ssDNA of (4-32) increased by 4 bases every run
• In two cases:
  – Carbyne alone
  – Carbyne with ssDNA

Approach
• First approach is using first principle simulation. Quantum ESPRESSO and its extension wannier90, open source codes, are used to calculate the band structure, quantum conductance, density of states, and current for the interaction between carbyne chains of different lengths and ssDNA
• Second approach is using molecular dynamic simulation (MD). NAMD, an open source code, is used to calculate the quantum conductance and tunneling current to scale the simulation up by including more ssDNA bases and evaluate the system in time.

Conclusion
• The band structure, quantum conductance, density of states, and current of different structures and lengths have been calculated.
• Bases A, G, C, and T of ssDNA have been included in two different structures. The band structure, quantum conductance, density of states, and current have been calculated and compared with the results when no amino acid included.
• Water molecule has been inserted within the structure that has chain of 16 carbon atoms attached to graphene sheets on both sides and base A to evaluate the difference.
• Input files and job scripts for MD simulations have been completed.

Next Steps
• MD simulation will be performed by following the same strategy. Quantum conductance and tunneling current will be calculated.