Molecular electronics and ultrafast DNA sequencing

Seung Kyu Min,[1] Kwang S. Kim[1]
[1] *Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Korea*

Delicate modulation of the molecular orbitals in molecular systems is useful to tune the performance of electron/spin transport. Not only electric and magnetic fields are powerful means for that purpose but also the characteristic change in conductance due to intermolecular interactions such as pi-pi stacking can be utilized for molecular sensing. Thus, we discuss the effects of external fields on molecular electronic and spintronic devices. Electron/spin transport phenomena in molecular electronic/spintronic devices [1] and graphene nanoribbon spin valves [2] are discussed based on density functional theory (DFT) coupled to non-equilibrium Green function theory (NEGF). The non-collinear spin states for the open systems are fully taken into account in a self-consistent manner with the non-equilibrium Green's function approach by using the Postrans program package [1-3]. A graphene nanoribbon (GNR) spin-valve device shows the super magnetoresistance behavior as a spin filter which selectively transmits almost 100% spin-polarized current [2]. Given that GNR electrodes show pristine molecular characteristics much better than Au or Ru electrodes [4], we find that measuring two-dimensional conductance spectra of a graphene [5] or GNR placed across a fluidic nanochannel leads to a powerful ultrafast DNA sequencing method [6]. In this device, while a single-stranded DNA (ssDNA) passes beneath the GNR, a single base interacts with the GNR via π-π stacking, giving a sharp conductance change. To explain the operation principle for sequencing the target ssDNA bases, we performed four step theoretical calculations. First, the binding energies between each DNA base and GNR are investigated from *ab initio* quantum chemical calculations. Second, the molecular dynamics study was performed in the realistic manner including the temperature effects, solvent molecules, and counter ions. Third, the electron transport properties of DNA base-GNR complex are studied by the DFT-NEGF method to understand the origin of conductance differences between DNA bases. Finally, we clarified the sequence of the target ssDNA via our data-mining technique and two-dimensional transient autocorrelation functions. This reliable ultrafast sequencing method would revolutionize the future bioinformatics and genetics.

[1] W. Y. Kim et al. *Acc. Chem. Res.* **43**, 111 (2010).
[2] W. Y. Kim et al. *Nature Nanotech.* **3**, 408 (2008).
[3] W. Y. Kim et al. *J. Comput. Chem.* **29**, 1073 (2008).
[4] Y. Cho et al. *J. Phys. Chem. A* **113**, 4100 (2009).
[5] K. S. Kim et al. *Nature* **457**, 706 (2009).
[6] S. K. Min, et al. *Nature Nanotech.* **6**, 162 (2011).