Asian Journal of Pharmaceutical Technology and Innovation

Abstract

Theoretical Investigation of Design Methodology, Optimized Molecular Geometries, and Electronic Properties of Benzene-Based Single Molecular Switch with Metal Nanoelectrodes

Rafsa Koyadeen T
BITS Pilani Dubai Campus, UAE

Abstract:

Understanding the electronic properties at the single molecular level is the first step in designing functional electronic devices using individual molecules. This paper proposes a simulation methodology for the design of a single molecular switch. A single molecular switch has two stable states that possess different chemical configurations. The methodology is implemented for 1,4-benzene dithiol (BDT) molecule with gold, silver, platinum, and palladium metal nanoelectrodes. The electronic properties of the designed metal-molecule-metal sandwich structure have been investigated using density functional theory (DFT) and Hartree-Fock (HF) method. It has been perceived that the DFT and HF values are slightly different as HF calculation does not include an electron-electron interaction term. Computation of the switching ratio gives the insight that BDT with gold has a high switching ratio of 0.88 compared with other three metal nanoelectrodes. Further, calculations of quantum chemical descriptors, analysis of the density of states (DOS) spectrum, and frontier molecular orbitals for both the stable states (i.e., ON and OFF state geometries) have been carried out. Exploring the band gap, ionization potential, and potential energy of two stable states reveals that the ON state molecule shows slightly higher conductivity and better stability than the OFF state molecule for every chosen electrode in this work. The proposed methodology for the single molecular switch design suggests an eclectic promise for the application of these new materials in novel single molecular nanodevices.

Biography:

Rafsa Koyadeen T is pursuing her PhD from Birla Institute of Technology and Science (BITS) Pilani, Dubai Campus in Nanoelectronics/Nanotechnology field. The above work has been done as a part of Rafsa's doctoral research at Birla Institute of Technology and Science (BITS) Pilani, Dubai Campus.It has been published recently in a peer reviewd international Journal: Journal of Nanomaterials in the month of Sep 2020.She has published 3 recent international journal papers and speaker at international conference held at Cambridge University,UK in 2016.

Publication of speakers:

1. A methedology to simulate and analyse molecules as molecular switches; S Devisree, A Kumar, RT Koyadeen.
2. Simulation and Analysis of BDT Molecule with Au Electrodes as a Molecular Switch; TR Koydeen, S Devisree, A Kumar, R Raj.

2nd Webinar on Nanotechnology and Nanomedicine, September 24, 2020, London, UK

Citation: Rafsa Koyadeen T; Theoretical Investigation of Design Methodology, Optimized Molecular Geometries, and Electronic Properties of Benzene-Based Single Molecular Switch with Metal Nanoelectrodes, United Arab Emirates; Nanomedicine 2020; September 24, 2020; London, UK.