Design and modelling of benzene based single molecular switches

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Abstract

Designed 1,4-benzene dithiol, 1,4-benzene diamine, and 1,4-benzene dicarboxylic acid based molecular switches with gold, silver, platinum and palladium metal electrodes by the first-principles approach. The electronic properties of the designed metal-moleculemetal sandwich structure are investigated with density functional theory (DFT) method. A series of benzene derivatives to explore the physical behaviour of conductance interpret in terms of nature of molecular backbone, anchoring group, contact geometry, nature of electrode material, molecular length, connectivity site, density of states, HOMO-LUMO gap, ionization potential and potential energy were systematically studied and compared. The findings of the present work clearly reveal that for the design of an efficient molecular switch, palladium and thiol are the best among electrode and anchoring group respectively. Palladium electrode shows high switching band gap ratio for ON and OFF state compared to Au, Ag, and Pt. The first principles approach can be used to screen and minimize the need for experimental approach which could be expensive.

Biography:

Rafsa Koyadeen T is pursuing Ph.D. from Birla Institute of Technology and Science (BITS) Pilani, Dubai Campus in the Material ScienceEngineering.She is currently working as a Research Scholar and Lab Engineer at Birla Institute of Technology and Science (BITS) Pilani, Dubai Campus for the past 2+years. She has published 3 recent international journal papers and speaker at international conference held at Cambridge University, UK in 2016.She is an active research scholar with recently published SCIE indexed 2 peer-reviewed international journal papers and 3+ years of teaching experience assisting and overseeing research projects with a Master's degree in Electronics and Communication Engineering. She is strongly focused on the ability to complete tasks accurately in a fast-paced environment with conflicting deadlines. She has proven abilities in academics and research in the field of Material Science, Chemistry and Physics with international conference speaker at Cambridge University, UK..

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