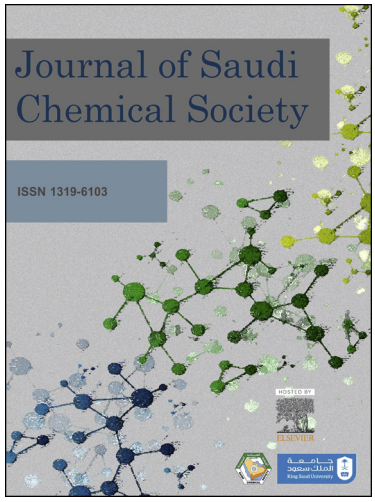

Original article

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Ayhan Üngördü, Nurten Tezer

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DFT study on metal-mediated uracil base pair complexes

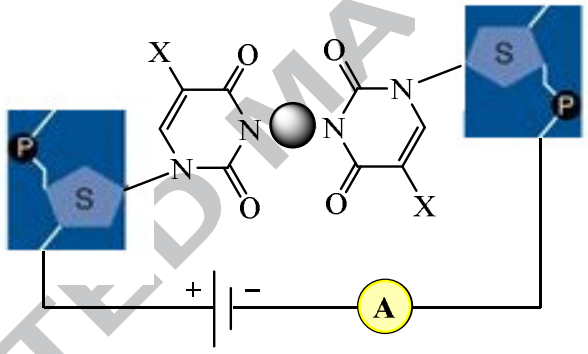
Ayhan ÜNGÖRDÜ & Nurten TEZER

aungordu@cumhuriyet.edu.tr

Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140, Sivas/TURKEY

Abstract

The most stable of metal-mediated uracil base pair complexes were determined. Method was used density functional theory, B3LYP. The calculations of systems containing C, H, N, O were described by 6-311++G(d,p) and cc-PVTZ basis sets and LANL2DZ and SDD basis sets was used for transition metals. Then Egap values of complexes were calculated and the electrical conductivity of the complexes for single nanowires were studied by band theory. Metal-mediated uracil base pair complexes which will used as conductive wires in nanotechnology were predicted. In nanoworld, this study is expected to show a way for practical applications.



Keywords electrical conductivity, metal-DNA, uracil, nanowires, DFT.

1. Introduction

Recently, DNAs and their derivatives have attracted much interest for the possibility of using such molecules as building blocks for electronic nano-devices (Scheme 1) [1-4]. Among these derivatives, metal-DNAs are obtained by treatment of DNA to metal ions [5]. Alkali (or rare-earth) ions form only electrostatic interactions with the nucleobases [6,7], but transition metal ions are expected to interact with the nucleobases also by chemical bonding [8-13]. However, transition metals are good carriers of many function particulary in the nanoworld. Thereof, they are also utilized for functionalization of DNA [14] among various modification schemes.