



Zahra Tavangar

Associate Professor

College: Faculty of Chemistry

Department: Physical Chemistry

Papers in Journals

1. Zahra Amaniseyed ,& Zahra Tavangar,Hydrogen storage on uncharged and positively charged Mg-decorated graphene,International Journal Of Hydrogen Energy,2019.
2. Z. Hajiahmadi ,& Z. Tavangar,Extensive theoretical study of corrosion inhibition efficiency of some pyrimidine derivatives on iron and the proposal of new inhibitor,Journal of Molecular Liquids,2019.
3. Zahra Hajiahmadi , Zahra Tavangar , Hadi Behzadi,A DFT Study of the Reaction between Benzopyrene Epoxide and C60 Derivatives as Possible Anticancer Activity,Polycyclic Aromatic Compounds,2019.
4. Seyedeh Leila Fani , Zahra Tavangar , Ali Kazempour,Boron decorated graphene nanosheet as an ultrasensitive sensor: the role of coverage,Journal of Molecular Modeling,2019.
5. A. Payvand ,& Z. Tavangar,Computational study on the functionalization of BNNC with pyrrole molecule,Superlattices and Microstructures,2018.
6. Z. Hajiahmadi ,& Z. Tavangar,Investigating the adsorption of nitrobenzene on M/Pd (1 1 1) bimetallic surface as an effective catalyst,Applied Surface Science,2018.
7. P. Mehdizadeh ,& Z. Tavangar,Photocatalyst Ag@N/TiO₂ nanoparticles: Fabrication, characterization, and investigation of the effect of coating on methyl orange dye degradation,Journal of Nanostructures,2017,ISC.
8. Z. Tavangar , M. Hamadianian , H. Basharnavaz,Studying the effects of the configuration of doped Al atoms on the conductive properties of boron nitride nanotube using density functional theory,Chemical Physics Letters,2017,ISI.
9. Z. Tavangar , M. Hamadianian , H. Basharnavaz,Variation of the electronic properties of zigzag boron nitride nanotubes by Al doping, A DFT study,Molecular Physics,2016,ISI.
10. M. Hamadianian Z. Tavangar S. Naseh,The modification of benzene adsorption on zigzag single-wall carbon nanotubes by carboxylation,Materials Research Express,2016.
11. M. Hamadianian , Z. Tavangar , S. Naseh,Improvement of electronic properties of carboxylated zigzag single wall carbon nanotubes by interaction with benzene derivatives,Current Applied Physics,2015.
12. M. Hamadianian , Z. Tavangar , B. Noori,Modification of conductive properties of (10, 0) zigzag single-walled carbon nanotubes (SWCNT) by alkali metals absorption,Journal of Molecular Structure,2014.
13. M. Hamadianian , Z. Tavangar , B. Noori,Modification of the electronic properties of zigzag (n = 5–10) and armchair (n = 3, 5) carbon nanotubes by K atom adsorption,Structal Chemistry,2014.
14. M. Hamadianian , Z. Tavangar , S. Naseh,The structural and electronic properties of (10,0) zigzag Single-Wall Carbon Nanotubes modified by thiophene groups,Chemical Physics Letters,2013.

15. Zahra Tavangar, Diels–Alder [4+2] Cycloadditions of C₂₀ with Some Diene and 1,2-Dioxo Compounds: A Theoretical Study, *Journal of Nanostructures*, 2012.
16. Zahra Tavangar, Diels–Alder [4+2] Cycloadditions of C₂₀ with Some Diene and 1,2-Dioxo Compounds: A Theoretical Study, *Journal of Nanostructures*, 2012.