به نام خدا

نام ونام خانوادگی : فرزانه فرزاد

زمینه مطالعاتی : شیمی فیزیک

زمینه تخصصی: کوانتوم و طیف سنجی

رتبه علمی : استادیار(دانشگاه روزانه بیرجند)

الف- تحصیلات

سال ۱۳۹۲ – اخذ دکتراي شيمي فيزيك ، دانشگاه بيرجند

سال ۱۳۹۵- استخدام به عنوان هیات علمی

ب ـ مقالات علمي منتشر شده در مجلات بين المللي معتبر علمي ـ پژوهشي

1. Probing the effect of polyethene glycol on the adsorption mechanisms of Gem on the hexagonal boron nitride as a highly efficient polymer-based drug delivery system: DFT, classical MD and Well-tempered Metadynamics simulations

April 2020Journal of Molecular Graphics and Modelling

Farzaneh FarzadHassan Hashemzadeh

2. Probing the adsorption and release mechanisms of cytarabine anticancer drug on/from dopamine functionalized graphene oxide as a highly efficient drug delivery system

March 2020Journal of Molecular Liquids

Maryam ZaboliHeidar RaissiNafiseh Rahmani MoghaddamFarzaneh Farzad

3. Assessment of adsorption behavior of 5-fluorouracil and pyrazinamide on carbon nitride and folic acid-conjugated carbon nitride nanosheets for targeting drug delivery

January 2020Journal of Molecular Liquids

Ameneh ZaboliHeidar RaissiFarzaneh FarzadHassan Hashemzadeh

4. Design of new materials based on functionalization of Cu-BTC for adsorption and separation of CH4 and CO2: GCMC and MD Simulations Study

December 2019Russian Journal of Physical Chemistry

Hassan HashemzadehHeidar RaissiFarzaneh Farzad

5. Molecular dynamics simulation study of Glycine tip-functionalisation of single-walled carbon nanotubes as emerging nanovectors for the delivery of anticancer drugs

October 2019Molecular Simulation

Zahra GhadriHeidar RaissiMahnaz Shahabi Ch.MFarzaneh Farzad

6. Enhance the efficiency of 5-fluorouracil targeted delivery by using a prodrug approach as a novel strategy for prolonged circulation time and improved permeation

July 2019International Journal of Pharmaceutics

Samaneh PasbanHeidar RaissiMajid PakdelFarzaneh Farzad

7. Using molecular dynamics simulation to explore the binding of the three potent anticancer drugs sorafenib, streptozotocin, and sunitinib to functionalized carbon nanotubes

June 2019Journal of Molecular Modeling

Narjes DehneshinHeidar RaissiZohre HasanzadeFarzaneh Farzad

8. Stabilization of D-lactate dehydrogenase diagnostic enzyme via immobilization on pristine and carboxyl-functionalized carbon nanotubes, a combined experimental and molecular dynamics simulation study

November 2018Archives of Biochemistry and Biophysics

Maryam ZaboliHeidar RaissiMahdiye Zaboli[...]Masoud Torkzadeh-Mahani

9. Monte Carlo simulation of CH 4 and CO 2 Adsorption and Separation in Single-Walled Carbon Nanotubes

September 2018First International Congress of Chemistry and Nanochemistry from Research to Technology

Hassan HashemzadehFarzaneh FarzadHeidar Raissi

10. Single-Walled Boron Nitride Nanotubes as Effective Adsorbent for Separation and Adsorption CO 2 and CH 4 : Monte Carlo Simulation

September 2018First International Congress of Chemistry and Nanochemistry from Research to Technology

Hassan HashemzadehHeidar RaissiFarzaneh Farzad

11. Monte Carlo simulation of CH 4 and CO 2 Adsorption and Separation in Single-Walled Carbon Nanotubes

September 2018First International Congress of Chemistry and Nanochemistry from Research to Technology

Hassan HashemzadehFarzaneh FarzadHeidar Raissi

12. Study on the interaction of Single-Walled Carbon Nanotube with organometallic transition metal compounds

August 2017The 6th International Conference of Chemistry, Chemical and Polymer Engineering

Maryam ZaboliHeidar RaissiFarzaneh Farzad

13. Investigating the pi – pi interaction between pyrazine and its different derivatives

August 2017The 6th International Conference of Chemistry, Chemical and Polymer Engineering

Maryam ZaboliHeidar RaissiFarzaneh Farzad

14. Investigation of the As, Ga, B and N-doped (6,0) aluminum phosphide nanotubes interactions with H2S gas: DFT study

August 20163rd conference on new Research achievements in chemistry and chemical engineering

Maryam ZaboliHeidar RaissiFarzaneh Farzad

15. Investigation the intermolecular hydrogen bonding between DNA thymine base dimer and its different derivatives

August 20163rd conference on new Research achievements in chemistry and chemical engineering

Maryam ZaboliHeidar RaissiFarzaneh Farzad

16. First-principles investigation of graphene sheet for sensing carbon dioxide

July 2016

Maryam ZaboliHeidar RaissiFarzaneh Farzad

17. First-principles investigation of graphene sheet for sensing carbon dioxide

July 2016

Maryam ZaboliHeidar RaissiFarzaneh Farzad

18. DFT study of the adsorption of H2S, H2Se and SO2 gas molecules on the surface of Fullerene

July 2016

Maryam ZaboliFarzaneh Farzad

19. Conformational, vibrational and electronic structure investigations of (z)-2-(oxosilyl) ethylenol

November 2014RSC Advances

Elahe MohammadinezhadH. RaissiFarzaneh Farzad

20. Quantum chemical studies on molecular conformations, energetic and intramolecular hydrogen bonding in ground and electronic excited state of (thioxosilyl) ethyleneselenol

March 2014Journal of Sulfur Chemistry

Farzaneh FarzadHossein FarsiHeidar Raissi

21. Theoretical investigation of substitution effect on the proton transfer mechanism in 3-mercapto-propenethial

August 2013Journal of Theoretical and Computational Chemistry

Heidar RaissiFarzaneh FarzadHossein Farsi

22. Conformational properties and intramolecular hydrogen bonding of 3-amino-propeneselenal: An ab initio and density functional theory studies

June 2013Journal of Theoretical and Computational Chemistry

Heidar RaissiFarzaneh FarzadShahira EslamdoostFariba Mollania

23. The effect of substitution on structure, intramolecular hydrogen bonding strength, electron density and resonance in 3-amino 2-iminomethyl acryl aldehyde

October 2012Journal of Theoretical and Computational Chemistry

Heidar RaissiMehdi YoosefianFariba MollaniaFarzaneh Farzad

24. Theoretical study on β-aminoacroleine; Density functional theory, atoms in molecules theory and natural bond orbitals studies

May 2012Journal of Chemical Sciences

Heidar RaissiMehdi YoosefianEffat MoshfeghiFarzaneh Farzad

25. Theoretical study of the effects of substitution, solvation, and structure on the interaction between nitriles and methanol

March 2012International Journal of Quantum Chemistry

Heidar RaissiFarzaneh FarzadEmad Saleh Nadim[...]Danial Loghmaninejad

26. Conformational study, molecular structure, and S..HN, S..HN intramolecular hydrogen bond in thioformyl-3-aminoacrylaldehyde

February 2012Journal of Sulfur Chemistry

Heidar RaissiMehdi YoosefianSoheila ZamaniFarzaneh Farzad

27. Theoretical Description of Substituent Effects in 2,4-Pentanedione: AIM, NBO, and NMR Study

January 2012Bulletin of the Chemical Society of Japan

Heidar RaissiMehdi YoosefianAhmad Hajizadeh[...]Farzaneh Farzad

28. Ab initio and DFT computational studies on molecular conformations and strength of the intramolecular hydrogen bond in different conformers of 3-amino-2-iminomethyl acryl aldehyde

June 2011Computational and Theoretical Chemistry

Heidar RaissiMehdi YoosefianFariba Mollania[...]Danial loghmaninejad

29. The effects of substitutions on structure, electron density, resonance and intramolecular hydrogen bonding strength in 3-mercapto-propenethial

November 2010Journal of Molecular Structure THEOCHEM

Heidar RaissiEmad Saleh NadimMehdi Yoosefian[...]Ali Amoozadeh

30. Ab initio and DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercapto-but-2-enethial

August 2010Journal of Sulfur Chemistry

Emad Saleh NadimHeidar RaissiMehdi Yoosefian[...]Alireza Nowroozi

31. Substituent Effect on Structure, Electron Density, and Intramolecular Hydrogen Bonding in Nitroso-Oxime Methane

January 2010International Journal of Quantum Chemistry

Mehdi YoosefianHeidar RaissiEmad Saleh Nadim[...]Alireza Nowroozi

32. Intramolecular Hydrogen Bond in 3-Imino-Propenylamine Isomers: AIM and NBO Studies

January 2009International Journal of Quantum Chemistry

H. RaissiAbraham F. JalboutB. Abbasi[...]Aned de Leon

33. Molecular structure and vibrational assignment of (trifluoroacetyl) acetone: A density functional study

April 2006Journal of Molecular Structure

Heidar RaissiAlireza NowrooziMozhgan RoozbehFarzaneh Farzad

34. Vibrational assignment, structure and intramolecular hydrogen bond study of 3-amino-1-phenyl-2-buten-1-one

April 2006Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy

Haidar RaissiAtieh YaraliFarzaneh FarzadAlireza Nowroozi

35. Vibrational assignment, structure and intramolecular hydrogen bond of 4-methylamino-3-penten-2-one

January 2006Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy

Heidar RaissiEffat MoshfeghiFarzaneh Farzad

36. Density functional theory study of the Fourier transform infrared and Raman spectra of Cu(II) bis-acetylacetone

December 2005Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy

Haidar RaissiAlireza NowrooziFarzaneh FarzadMohammad saeid Hosseini

37. The presentation of an approach for estimating the intramolecular hydrogen bond strength in conformational study of β-Aminoacrolein

October 2005Journal of Molecular Structure THEOCHEM

Alireza NowrooziHaidar RaissiFarzaneh Farzad

38. Vibrational assignment and structure of 3-(4-methoxyphenyl)pentane-2,4-dione

October 2005Journal of Molecular Structure

Heidar RaissiFarzaneh FarzadAlireza Nowroozi