CURRICULUM VITAE

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نام و نام خانوادگی: احسان زاهدی

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آدرس و تلفن محل کار: شاهرود-دانشگاه آزاد- دانشکده علوم پایه- گروه شیمی

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تلفن همراه: ۰۹۱۲۲۷۳۳۷۵۵-۰۹۳۹۲۷۳۳۷۵۵

سوابق تحصیلی:

- کارشناسی شیمی کاربردی-دانشگاه آزاد شاهرود-سال ۱۳۷۸
- کارشناسی ارشد شیمی فیزیک- دانشگاه آزاد شاهرود-سال ۱۳۸۲
- دکترای شیمی فیزیک- دانشگاه آزاد علوم و تحقیقات تهران-سال ۱۳۸۶

سوابق اجرائی و مدیریتی

- مدیر گروه کارشناسی و کارشناسی ارشد گروه شیمی ۱۳۹۰-۱۳۸۷
- مدیر گروه کارشناسی ارشد مهندسی شیمی ۱۳۸۸-۱۳۸۹
- عضو شورای تحصیلات تکمیلی ۱۳۸۸تا کنون
- عضو کمیته مشورتی پژوهشی ۱۳۹۲ تا کنون

افتخارات علمی و پژوهشی:

- پژوهشگر برتر در سال ۱۳۹۰
- پژوهشگر برتر در سال ۱۳۹۱
- پژوهشگر برتر در سال ۱۳۹۲

سوابق پژوهشی:

- **لیست مقالات ISI**

1. "Solvent effects on stability and ^{15}N NMR shielding of 5-methylcytosine tautomers:A theoretical approach" *Journal of Molecular Structure: THEOCHEM*.

   E. Zahedi*, M. Aghaie, K. Zare, H. Aghaie. 2009.

2. "A density functional study of NBO, NICS and ^{14}N NQR parameters of 5-methyl-cytosine tautomers in the gas phase" *Journal of Molecular Structure: THEOCHEM*.

   E. Zahedi*, M. Aghaie, K. Zare. 2009.

3. "NBO and NICS analysis of the allylic rearrangements (the Cope and 3-aza-Cope rearrangements) of hexa-1,5-diene and N-vinylprop-2-en-1-amine: A DFT study" *Central European Journal of Chemistry*.

   E. Zahedi*, S. Ali-Asgari, V. Keley. 2010.

4. "Kinetic and thermodynamic study of the substituent effect on the amino-Claisen rearrangement of para-substituted N-allyl-N-arylamine: a Hammett study via DFT" *Molecular Simulation.*

   S.R. Emamian, M. Aghaie*, M.R. Zardoost, E. Zahedi, K. Zare. 2010.

5. "Theoretical study of HF elimination kinetics of ethane fluorides and derivatives [C2H6-*n*F*n* (*n* = 1- 4)]" *Indian Journal of Chemistry.*

   A. Shiroudi*, E. Zahedi. 2010.

6. "Control aromaticity in the thermal decomposition of 2,5-dihydrofuran, 2,5-dihydrothiophene and 3-pyrroline: a kinetic and thermodynamic study via DFT" *Reaction Kinetic Mechanism Catalysis*.

   A. Shiroudi, E. Zahedi*, R. Zabihi. 2011.

7. "A DFT study of NBO and NICS analysis of the allylic rearrangements (the Claisen and thio-Claisen rearrangements) of 3-(vinyloxy)prop-1-ene and allyl vinyl sulfide" *Phosphorus, Sulfur, and Silicon and the Related Elements.*

   E. Zahedi*, A. Shiroudi, S. Ali-Asgari, V. Keley. 2011.

8. "The influence of NH_3-attaching on the NMR parameters in the zigzag BN nanotube" *Superlattices and Microstructures.*

   E. Zahedi, A. Bodaghi, A. Seif*, A. Boshra. 2011.

9. "Mechanism and regioselectivity of the 1,3-dipolar cycloaddition of methyleneamine N-oxide with cyclopent-3-ene-1,2-dione and its aza, oxa and thia analogs: A DFT approach" *Progress in Reaction Kinetics and Mechanism*.

S.R. Emamian, E. Zahedi*. 2012.

10. "Structural and electronic properties of ammonia adsorption on the $C_{30}B_{15}N_{15}$ heterofullerene: A DFT study" *Journal of Computational and Theoretical Nanoscience*.

E. Zahedi*, A. Seif, T.S. Ahmadi. 2011.

11. "Thermal Decomposition Kinetics of Ethane Halides and Derivatives [$C_2H_{6-n}X_n$ (n=1-3); X= F, Cl, Br]: DFT Study and NBO Analysis" *Chinese Journal of Structural Chemistry*.

A. Shiroudi*, E. Zahedi. 2011.

12. "DFT study of the allylic rearrangements (the Cope rearrangements) of substituted hexa-1,5-dienes: NBO and NICS analysis" *Progress in Reaction Kinetics and Mechanism*.

H. Aghaie*, E. Zahedi, S. Mohammadkhani, M. Aghaie. 2011.

13. "Theoretical study and NBO analysis on the gas phase elimination kinetics mechanism of 2-chloroethylsilane and derivatives" *Progress in Reaction Kinetics and Mechanism*.

A. Shiroudi*, E. Zahedi. 2012.

14. "A theoretical study of NBO, NICS and ^{14}N NQR parameters of adenine tautomers in the gas phase via DFT" *Journal of Heterocyclic Chemistry*.

E. Zahedi*. 2012.

15. "Ammonia adsorption on the $C_{30}B_{15}N_{15}$ heterofullerene: DFT study of nuclear magnetic shielding and electric field gradient tensors of N and B nuclei" *Journal of Physica B: Condensed matter*.

E. Zahedi*. 2011.

16. "Adsorption of NH_3 and NO_2 molecules on $C_{48}B_6N_6$ heterofullerene: A DFT study on electronic properties" *Journal of Physica B: Condensed matter*.

E. Zahedi*, A. Seif. 2011.

17. "Size-dependent electronic structures of boron carbonitride (BC2N) nanotubes. A DFT approach" *Superlattices and Microstructures*.

E. Zahedi*. 2011.

18. "The comparative study in transport properties of furan,thiophene and selenophene dithiols in nano electronic" *Superlattices and Microstructures*.

E. Zahedi*, A. Pangh. 2011.

19. "Effect of tube radius on the electronic and magnetic properties of finite boron nitride zigzag nanotubes using DFT" *Journal of Physica E: Low-dimensional Systems and Nanostructures*.

E. Zahedi*, A. Seif. 2011.

20. "A DFT study of carbon nanobuds" *The European Physical Journal B.*

A. Seif*, E. Zahedi, T.S. Ahmadi. 2011.

21. "Characterization of a redox-responsive molecular switch based on dibenzo[1,2] dithiine using DFT" *Chinese Journal of Structural Chemistry*.

E. Zahedi*, S.R. Emamian, A. Shiroudi. 2012.

22. "DFT Calculations and NBO Analysis of 2-chloroethylethyldichlorosilane Unimolecular Elimination Kinetics in the Gas Phase" *Chinese Journal of Structural Chemistry*.

A. Shiroudi*, E. Zahedi. 2012.

23. "Kinetic study and NBO analysis of the dehydrogenation mechanism of five-membered ring heterocyclic 2,5-dihydro-[furan, thiophene, selenophene]" *Chinese Journal of Chemistry*.

A. Shiroudi*, E. Zahedi. 2011.

24. "Ab initio study and NBO analysis of the unimolecular decomposition kinetics of 2,2-dimethyloxetane" *Progress in Reaction Kinetics and Mechanism.*

A. Shiroudi*, E. Zahedi. 2012.

25. "Theoretical study of kinetics and thermodynamics of hetero Diels-Alder reaction of thiazole and isothiazol with thiophene-2,5-dione "*Chinese Journal of Structural Chemistry*.

S.R. Emamian, J. Nabavi, F. Shams, E. Zahedi*. 2011.

26. " A computational investigation of carbon-doped beryllium monoxide nanotubes" *Central European Journal of Chemistry*.

A. Seif*, E. Zahedi, G.M. Rozbahani. 2012.

27. "A DFT studies of structural and quadrupole coupling constants properties in C-doped BeO nanotubes" *Superlattices and Microstructures.*

A. Seif*, E. Zahedi. 2011.

28. "The unimolecular thermal decomposition of Oxetane and methyl derivatives: An ab initio and RRKM calculations" *Russian Journal of Physical Chemistry A.*

A. Shiroudi*, A. Tahan, E. Zahedi. 2012.

29. "DFT study of NBO, NICS and ^{14}N NQR parameters of guanine tautomers in the gas phase" *Zeitschrift für Physikalische Chemie.*

E. Zahedi*, K. Zare, H. Aghaie, S.R. Emamian, A. Shiroudi. 2012.

30. "DFT calculations of the elimination kinetics of silacyclobutanes and its methyl derivatives in the gas-phase" *Phosphorus, Sulfur, and Silicon and the Related Elements*.

A. Shiroudi*, E. Zahedi. 2012.

31. "Exohedral chemical functionalization of $C_{48}B_6N_6$ with NH_3: Binding energies and electronic structures of $C_{48}B_6N_6$–$(NH_3)_{n=1-6}$" *Superlattices and Microstructures*.

E. Zahedi*, A. Seif. 2012.

32. "Mechanism and regioselectivity of the 1,3-dipolar cycloaddition of thiocarbonyl S-imide with cyclopent-3-ene-1,2-dione and methoxyethene: A DFT approach" *Physical Organic Chemistry*.

S.R. Emamian*, E. Zahedi. 2012

33. "Effect of tube radius on the exohedral chemical functionalization of boron-nitride zigzag nanotubes with NH_3" *Journal of Physica B: Condensed matter*.

E. Zahedi*. 2012.

34. "The allylic rearrangements (Claisen and thio-Claisen) and decomposition reactions of allylformate and sulfur analogue: DFT study and NICS analysis" *Progress in Reaction Kinetics and Mechanism*.

A. Shiroudi*, E. Zahedi. 2013.

35. "Theoretical study of the pressure dependent rate constants of the thermal decomposition of β-propiolactone" *Arabian Journal of Chemistry*.

A. Shiroudi*, E. Zahedi. Accepted for Publication.

36. "Ab initio and RRKM study of the unimolecular decomposition of five- membered ring heterocyclic (X= O, S, N-H)" *Chinese Journal of Structural Chemistry*.

A. Shiroudi*, E. Zahedi. 2012.

37. "DFT-NEGF study of transport properties and NDR behavior in fused furan and thiophene dimmers" *Journal of Physica B: Condensed matter*.

E. Zahedi*. 2012.

38. "Isomerization reactions of α-methyl allyl [acetate (1), trifluoro acetate (2)]: A Theoretical (NBO, NICS, RRKM) Study" *Progress in Reaction Kinetics and Mechanism*.

A. Shiroudi*, E. Zahedi. 2013.

39. "Adsorption of nitrogen dioxide on $C_{30}B_{15}N_{15}$ heterofullerene: AIM and NBO study via DFT" *Comptes Rendus Chimie*.

E. Zahedi*. 2013.

40. "Theoretical study of proton transfer in ammonia-hydrogen halides in the presence of methanol" *Research on Chemical Intermediates.*

A. Pangh*, E. Zahedi. 2013.

41. "DFT study of the mechanism and regioselectivity of 1,3-pentadiene with methyl acrylate using theoretical approaches" *Chinese Journal of Structural Chemistry*.

A. Shiroudi*, E. Zahedi. 2013.

42. "The influence of NO2-attaching on the nuclear magnetic shielding tensors of N and B nuclei in $C_{30}B_{15}N_{15}$ heterofullerene: A DFT study" *Research on Chemical Intermediates.*

E. Sedghamiz, Z. Halfinezhad, A. Shiroudi, E. Zahedi*. 2013.

43. "Comparative investigation of stability of indene and isoindene and the their heteroanalogs (N,O,S) using the computational methods" *Phosphorus, Sulfur, and Silicon and the Related Elements.*

S. Ali-Asgari*, E. Zahedi, S.R. Emamian. Accepted for publication.

44. "Mechanism and regioselectivity of 1,3-dipolar cycloaddition reactions of sulfur-centered dipoles with furan-2,3-dione: a theoretical study using DFT" *Journal of Chemical Sciences.*

S.R. Emamian*, S. Ali-Asgari, E. Zahedi. 2014

45. "DFT study of electric field effects on the isomerization of a photochromic molecular switch based on 1,2-dithienylethene" *Canadian Journal of Chemistry*

E. Zahedi*, M. Mozaffari, F-S. Karimi, A. Nouri. 2014.

46. "Current-voltage characteristics through dithienylcyclopentene: A NEGF-DFT study" *Journal of Physica E: Low-dimensional Systems and Nanostructures*.

E. Zahedi*, A. Pangh. 2014.

47. "DFT study of hydrogen storage on Li- and Na- doped $C_{59}B$ heterofullerene" *Surface Review and Letters.*

E. Zahedi*, M. Mozaffari. 2014

48. "Diels-Alder reactions of α-cyano α,β-unsaturated ketones with 2-methyl-1,3-butadiene: DFT study of mechanism, reactivity and regioselectivity" *International Journal of Chemical Kinetics*

A. Nouri*, E. Zahedi, F. Joneydi Jafari. Accepted

49. "Molecular dynamics simulation of boron nitride nanotube as a drug carrier " *Arabian Journal for Science and Engineering*

E. Sedghamiz, E. Jamalizadeh, S.M.A Hosseini*, T. Sedghamiz, E. Zahedi . 2014

50. "Mechanism and regioselectivity of the reversible Diels-Alder cycloaddition of 2-methyl-1,3 butadiene with $C_{48}B_6N_6$ heterofullerene: A DFT approach" *Molecular Graphics and Modelling*

E. Zahedi*. 2014

51. "DFT study of CO and NO adsorption on boron nitride $(BN)_{n=3-5}$ nano clusters" *Surface Review and Letters.*

E. Zahedi, A. Pangh*, H. Ghorbanpour. Accepted

- **لیست مقالات ISI تحت داوری**

52. "Hydrostatic pressure on the electronic and optical properties of the bulk and nano-ribbon Bi_2S_3: A DFT study" *Computational Material Science*

E. Zahedi*

53. "DFT study of structural, elastic properties and thermodynamic parameters of Bi_2S_3 ribbons under hydrostatic pressures" Journal of Physics: Condensed Matter

E. Zahedi*, B. Xiao

- **لیست مقالات ISC**

54. "Ab initio and DFT studies on tautomerism of 5-methylcytosine in gaseous phase", *J. Phys. Teor. Chem. IAU,* 2007.

Karim Zare, Majid Monajjemi, Ehsan Zahedi, Hossein Aghaie*

55. "A Theoretical Study on Aromaticity of 5-methylcytosine tautomers in gas phase", *J. Phys. Teor. Chem. IAU,* 2008.

H. Aghaie*, K. Zare, E. Zahedi, S.R. Emamian

56. "Kinetic and thermodynamic study of the substituent effect on the Claisen rearrangement of para-substituted allyl aryl ether: a Hammett study via DFT" *J. Phys. Teor. Chem. IAU,* 2009.

S.R. Emamian, M.R. Zardoost, K. Zare, E. Zahedi, H. Aghaie*

57. "A density functional theory study of the regio selectivity of the Diels –Aldercyclo addition of 2 methyl- substituted diene with selected dienophiles" *J. Phys. Teor. Chem. IAU,* 2013.

A. Nouri*, E. Zahedi, F. Joneydi Jafari, S. Sedaghat

58. "Impact of Lewis acid catalyst on the regioselectivity and kinetics of 1,3-dipolar cycloaddition reaction of azidobenzene with acrolein: a theoretical study using DFT" *J. Phys. Teor. Chem. IAU*, 2013.

F. Shams, S.R. Emamian*, E. Zahedi

- **لیست مقالات سمینارهای بین المللی**

59. "A Novel Pathway for the Preparation of Mesoporous Si-MCM-41, and Its Characterization" 2nd International Congress On Nanoscience & Nanotechnology (ICNN2008), October, 2008, Tabriz, Iran.
60. "Synthesis of Pt/Pd/Bi Nanoparticles in MCM-41 Host under Alkaline Conditions, and Its Characterization" 2nd International Congress On Nanoscience & Nanotechnology (ICNN2008), October, 2008, Tabriz, Iran.

- **لیست مقالات سمینارهای ملی (تحت نظر انجمن شیمی ایران)**

61. "NBO Study of Para derivatives of methoxy- and trifluoromethoxy Benzene with different torsion angles", 10th Iranian Physical Chemistry Seminar, April, 2007, Isfahan, Iran.
62. "Nucleus-Independent Chemical Shifts (NICS) Criterion to Evaluate Aromaticity in para-Substituented Phenol with Different Torsion Angles", 14th Iranian Organic Chemistry Seminar, March, 2008, Zabol, Iran.
63. "NBO Analysis and Electronic Structure of Heterocyclic Ring in XTC", 14th Iranian Organic Chemistry Seminar, March, 2008, Zabol, Iran.
64. "Computational Study on the Kinetic of 3-Aza-Cope Rearrangement in the Gas Phase", 14th Iranian Organic Chemistry Seminar, March, 2008, Zabol, Iran.
65. "NBO Analysis of Intramolecular Hydrogen Bond in Bis-4-amino-3-pentene-2-one" 15th Iranian Seminar of Organic Chemistry (15ISOC), August, 2008, Kermanshah, Iran.
66. "Solvent effects on stability and ^{15}N NMR shielding of XTC" 15th Iranian Seminar of Organic Chemistry (15ISOC), August, 2008, Kermanshah, Iran.
67. "Substituent Effects in the Synthesis of Thioureas from Reaction of Anilines with Benzoylisothiocyanate: A Hammett Study via DFT Method" 15th Iranian Seminar of Organic Chemistry (15ISOC), August, 2008, Kermanshah, Iran.

68. "Synthesis of Bis-4-amino-3-pentene-2-one and Study on Interamolecular Hydrogen Bond" 15th Iranian Seminar of Organic Chemistry (15ISOC), August, 2008, Kermanshah, Iran.
69. "The Kinetic and Thermodynamic Study on the Claisen Rearrangement in the Gas Phase Using Computational Calculations" 15th Iranian Seminar of Organic Chemistry (15ISOC), August, 2008, Kermanshah, Iran.
70. "Substituent study on 1, 3-D.C. of substituted nitrones with ethylene: a Hammett study via DFT" 17th Iranian Seminar of Organic Chemistry, October, 2010, Babolsar, Iran.
71. "Substituent effect on Baeyer–Villiger oxidation of substituted benzaldehydes with ethaneperoxidacid: A Hammett study via DFT" 17th Iranian Seminar of Organic Chemistry, October, 2010, Babolsar, Iran.
72. "Electrophilic addition of hydrogen fluoride and water to asymmetric olefins:A DFT study" 17th Iranian Seminar of Organic Chemistry, October, 2010, Babolsar, Iran.
73. "Theoretical study of the mechanism, regio- and stereoselectivity of the Diels–Alder reaction of para-substituted 1-phenyl-1,3-cyclopentadiene with cyclopent-2-enone" 17th Iranian Seminar of Organic Chemistry, October, 2010, Babolsar, Iran.
74. "Substituent effects in the Diels–Alder reaction of para- substituted 2-phenylfuran with crotonolactone: A Hammett study via DFT" 17th Iranian Seminar of Organic Chemistry, October, 2010, Babolsar, Iran.
75. "DFT study on a selective BN- doped graphene" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
76. "Effect of B and Al functional groups on a selective graphene: A computational study" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
77. "The comparative study of transport properties of furan, thiophene and selenophen dithoils in Nano Electronics" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
78. "Theoretical study of hydrogen storage in Li–ethylene complex via DFT" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
79. "Aromaticity analysis of stable guanine tautomers in the gas phase via DFT" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.

80. "The NO2 adsorption on the C48B12 heterofullerene: DFT study of B electric field gradient tensors" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
81. "Electric field effects on the switching of molecular switch via DFT" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
82. "The NO2 attached C30B15N15 heterofullerene: A Computational Nuclear Magnetic resonance study" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.
83. "Hydrohalogenation and hydration of asymmetric olefins: a DFT study" 14th Iranian Physical Chemistry Conference, February, 2011, University of Tehran-Kish, Iran.