

Fatemeh Ektefa



Assistant Professor of Physical Chemistry,
Department of Chemistry, Faculty of Science,
Shahid Rajaee University, Tehran, Iran
(Since 23/09/2023)

Education

Ph.D:

Physical Chemistry (Sep. 2012 – Feb. 2018)

Tarbiat Modares University, Tehran, Iran

Total GPA: 18.78 (out of 20)

Dissertation: "Study of adsorption and diffusion of hydrocarbon compounds in nano channels of zeolites: computational aspect"
Supervised by Dr. Soheila Javadian Farzaneh

Sabbatical period:

Department of Chemistry, **University of British Columbia (UBC)**, Vancouver, Canada (Feb. 2016- Sep. 2016)

Project: "Computational comparison of efficiency of zeolites as drug delivery systems for cancer drugs"
Supervised by Dr. Yan Alexander Wang

M.Sc:

Physical Chemistry (Sep. 2008 – Feb. 2010)

Tarbiat Modares University, Tehran, Iran

Total GPA: 17.72 (out of 20)

Dissertation: "Structural study and determination of NMR and NQR parameters in azobenzene nanobioswitch using computational chemistry methods."
Supervised by Prof. N. L. Hadipour

B.Sc:

Pure Chemistry (Sep. 2003 – Jul. 2007)

Alzahra University, Tehran, Iran

Total GPA: 16.04 (out of 20)

CONTACT

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Google scholar Profile:

https://scholar.google.com/citations?use_r=midvigoAAAAJ&hl=en

✓ **RESEARCH INTERESTS-----**

✓ **Computational Chemistry**

1- Molecular Simulation of:

- Adsorption, Separation and Purification of Gases and Pollutants Removal from Wastewater by Nanoporous Materials
- Nano-Confining Fluids,
- Two-Dimensional Nanostructures,
- Molecular Switches,
- Biomolecules and Drugs,

2- Quantum Chemical Calculations of mentioned systems aimed to provide Deeper Insight of Guest-Host Chemistry

❖ Chemometrics

✓ **RESEARCH PROJECTS-----**

- “Biomedical Applications of Zeolites: Computational Study”, Dr. Yan Alexander Wang’s group, **UBC, Vancouver, Canada** (2016)
- **Postdoctoral Researcher**, Dr. Jafar Towfighi’s group, **Department of Chemical Engineering, Tarbiat Modares University**, Tehran, Iran (2018-2019)
- “Industrial Applications of Zeolites: Computational Study”, Dr. Jafar Towfighi’s group, **Department of Chemical Engineering, Tarbiat Modares University & INSF**, Tehran, Iran (2019-2020)

✓ **TEACHING EXPERIENCE-----**

❖ **Working in the position of Academic Teacher:**

- Advanced Physical Chemistry, Physical Chemistry I & II, General Chemistry, Industrial chemistry, Basic Principles and Calculations in Chemical Engineering and HSE courses at graduate & under graduate levels, **Khatam Alanbia Technology University**, Behbahan, Khuzestan, Iran (2016-2023).
- Physical Chemistry, Thermodynamics of Chemical Engineering, and General Chemistry courses at graduate level, **Shahre Ghods branch of Islamic Azad University**, Tehran, Iran (2013- 2017)
- Physical Chemistry and Advanced Physical Chemistry courses at graduate level, **Tehran shargh branch of Islamic Azad University**, Tehran, Iran (2014- 2015)
- Chemistry courses at **University of Applied Science and Technology**, Tehran, Iran (2012, Feb-Jul)
- Teaching Assistant in Quantum chemistry II & III, Statistical thermodynamics, Chemical kinetic at **Tarbiat Modares University**, Tehran, Iran (2015-2017)
- Holding problem solving course for Advanced Physical Chemistry in the academic years.

❖ **Working in the position of Advisor:**

- Advising for MS thesis, **Khatam Alanbia Technology University**, Behbahan, Khuzestan, Iran (2021-2022).
- Advising for MS thesis, **Shahre Ghods branch of Islamic Azad University**, Tehran, Iran (2013-2014).

❖ **Working in the position of Teacher:**

- Chemistry course at **high School**, Behbahan, Khuzestan, Iran.
- Chemistry course at **high School**, District 1, Tehran, Iran.

✓ PROFESSIONAL EXPERIENCE-----

- ❖ **Research Institute of Petroleum industry of Iran (RIPI), Tehran, Iran** (Jan. 2011-2022)
The accomplished projects were as follows: Computational study on the zeolites
- ❖ **Food, Drug and Medical Equipment Control Reference Laboratories, Tehran, Iran**
Quality Control Expert and Researcher of Cosmetic Department (Apr. 2008- Jul. 2009)

✓ HONORS and AWARDS-----

- ❖ Ranked 1st based on overall GPA among the Ms. graduate students in the field of Physical Chemistry, Department of Chemistry, Tarbiat Modares University (Feb. 2010)
- ❖ 11th rank at the national entrance exam of the state universities for Ph.D degree (Sep. 2012)
- ❖ Awarded the Ministry of Science of Iran scholarship for Ph.D sabbatical leave in University of British Columbia (UBC), Vancouver, Canada (2016)
- ❖ Ranked 1st based on overall GPA among the Ph.D graduate students in the field of Physical Chemistry, Department of Chemistry, Tarbiat Modares University (Feb. 2018)
- ❖ The Best Researcher of the Young Researchers Club (2018)
- ❖ Received Teaching Qualification Certificate from Tarbiat Modares University (2018)
- ❖ Postdoctoral fellowship, by Iran National Science Foundation (INSF), Tehran, Iran (2018)
- ❖ Received an Academic Award from Iran's National Elites Foundation (INEF) (2023)

✓ PUBLICATION-----

❖ Journal Articles

1. **F. Ektefa**, Z. Khodadadi, F. Naderi, F. Fathi, “[A computational evidence of the intermolecular hydrogen bonding in leflunomide: Chemical shielding tensors](#)”, *Computational and Theoretical Chemistry*, 2023, 1221, 114027. <https://doi.org/10.1016/j.comptc.2023.114027>
2. **F.Ektefa**, J. Towfighi, S. Soltanali, “[Performance of BEA, FAU, LTL, MFI, and MOR zeolites in the removal of ethyl mercaptan traces from natural gas by Monte Carlo molecular simulation](#)”, *Applied Surface Science*, 2022. <https://doi.org/10.1016/j.apsusc.2022.154833>
3. S. Javadian, K. Najafi, M. Sadrpoor, **F. Ektefa**, N. Dalir, M. Nikkhah, “[Graphene quantum dots based magnetic nanoparticles as a promising delivery system for controlled doxorubicin release](#)”, *Journal of Molecular Liquids*, 2021, 331, 115746. <https://doi.org/10.1016/j.molliq.2021.115746>
4. **F. Ektefa**, S. Javadian, M. Rahmati, “[Computational comparison of the efficiency of nanoporous zeolite frameworks for separation of phenol from water](#)”, *Journal of the Taiwan Institute of Chemical Engineers*, 2018, 88, 104–113. <https://doi.org/10.1016/j.jtice.2018.03.020>
5. M. Mahdavian, A. R. Tehrani-Bagh, E. Alibakhshi, S. Ashhari, M. J. Palimi, S. Farashi, S. Javadian, **F. Ektefa**, “[Corrosion of mild steel in hydrochloric acid solution in the presence of two cationic gemini surfactants with and without hydroxyl substituted spacers](#)”, *Corrosion Science*, 2018, 137, 62–75. <https://doi.org/10.1016/j.corsci.2018.03.034>
6. M. Anafcheh, F. Naderi, Z. Khodadadi, **F. Ektefa**, R. Ghafouri, “[Exploring Adjacent Pentagons in Non-IPR and SW Defective Si60 and Si70 Silicon Fullerenes: a Computational Study](#)”, *Silicon*, 2019, 11, 323-329. [10.1007/s12633-018-9994-x](https://doi.org/10.1007/s12633-018-9994-x)

22. R. Ghafouri and **F. Ektefa**, "Functionalization of carbon ad-dimer defective single-walled carbon nanotubes through 1,3-dipolar cycloaddition: a DFT study", *Structural Chemistry*, 2015, 26, 507-515. <https://doi.org/10.1007/s11224-014-0507-2>
23. F. Naderi, R. Ghafouri and **F. Ektefa**, "1,3-Dipolar Cycloaddition in Stone-Wales Defective Carbon Nanotubes: A Computational Study", *Journal of Cluster Science*, 2015, 26, 581-594. <https://doi.org/10.1007/s10876-014-0827-9>
24. M. Zahedi-Tabrizi and **F. Ektefa**, "A computational evidence of the intermolecular/intramolecular hydrogen bonding in Salicylsalicylic acid: chemical shielding tensors and AIM analysis", *Monatshefte fur Chemie*, 2015, 146, 1837-1843. <https://doi.org/10.1007/s00706-015-1466-z>
25. H. Djahaniani, F. Fatemi, **F. Ektefa**, B. Mohtat, and B. Notash, "Green Approach to Stereoselective Synthesis of Benzo[d]chromeno[3,4-h]oxathiazonine Derivatives via MCRs in Water: A Combined, Experimental and DFT Study", *Combinatorial Chemistry & High Throughput Screening*, 2015, 18, 990-999. <https://doi.org/10.2174/1386207318666150915113230>
26. S. Soltanali, R. Halladj, and **F. Ektefa**, "A DFT Exploration of the Adsorption of Methanol on the Brönsted Acid Site of Nanostructured H-ZSM-5 Catalyst: Probing the Effect of Cluster Size on the O-H...O Hydrogen Bond Based on NMR and NQR Parameters", *Journal of Cluster Science*, 2015, 26, 565-579. <https://doi.org/10.1007/s10876-014-0839-5>
27. M. Bozorg, T. Shahrabi Farahani, J. Neshati, G. Mohammadi Ziarani, Z. Chaghazardi, P. Gholamzade, and **F. Ektefa**, "Corrosion inhibitive behavior of 7-hydroxyphenoxazole on mild steel in 1.0 M HCl", *Research on Chemical Intermediates*, 2015, 41, 6057-6071. <https://doi.org/10.1007/s11164-014-1722-6>
28. S. Soltanali, R. Halladj, and **F. Ektefa**, "A computational exploration into isomorphously substituted effects on hydrogen electric field gradient and chemical shielding tensors in the H-ZSM-5 zeolite", *Asia Pacific Journal of Chemical Engineering*, 2014, 9, 574-580.
29. M. Bozorg, T. F. Shahrabi, G. Z. Mohammadi, J. Neshati, Z. Chaghazardi, P. Gholamzadeh, and **F. Ektefa**, "Inhibitive assessment of N-(8-bromo-3H-phenoxazin-3-ylidene)-N,N'-dimethylaminium, as a novel corrosion inhibitor for mild steel in 1.0 M HCl", *Journal of Advanced Materials and Processing*, 2014, 2(3), 27-38.
30. F. Fathi, **F. Ektefa**, K. Sohrabzadeh, A. Arefi-Oskouie, M. Tafazzoli, K. Rostami, M. R. Zali, and M. Rostami-Nejad, "A Metabonomics Study on Celiac Disease by CART", *International Journal of Celiac Disease*, 2014, 2, 44-46.
31. F. Fathi, **F. Ektefa**, M. Tafazzoli, K. Rostami, M. R. Nejad, M. Fathi, M. Rezaye-Tavirani, A. A. Oskouie, and M. R. Zali, "The concentration of serum zinc in celiac patients compared to healthy subjects in Tehran", *Gastroenterology and Hepatology from Bed to Bench*, 2013, 6, 92-95.
32. F. Fathi, **F. Ektefa**, A. Arefi Oskouie, K. Rostami, M. Rezaei-Tavirani, A. Houshang, M. Alizadeh, M. Tafazzoli, M. Rostami Nejad, "NMR based metabonomics study on celiac disease in the blood serum", *Gastroenterology and Hepatology from Bed to Bench*, 2013, 6, 190-194.
33. F. Fathi, **F. Ektefa**, M. Hagh-Azali, and H. A. Aghdaie, "Metabonomics exposes metabolic biomarkers of Crohn's disease by 1HNMR", *Gastroenterology and Hepatology from Bed to Bench*, 2013, 6, S19-S22.
34. A. Mortazavi, **F. Fathi**, F. Ektefa, M. Tafazzoli, A. Arefi oskouie, M. Rezaie-Tavirani, M. R. Zali, M. Rostami Nejad, and K. Rostami, "Investigation of metabonomics technique by analyze of NMR data, which method is better? Mean center or auto scale?", *Journal of Paramedical Sciences (JPS)*, 2013, 4, 1-10.
35. **F. Ektefa**, M. Anafche, and N. L. Hadipour, "A DFT exploration of structural and electronic properties of a photoswitchable octapeptide cyclized with (4-aminomethyl)phenylazobenzoic acid", *Computational and Theoretical Chemistry*, Dec 2011, 977, 1-8. <https://doi.org/10.1016/j.comptc.2011.07.023>

36. F. Fathi, A. Arefi Oskouie, N. Naderi, Z. Kariminia, S. Fathi, **F. Ektefa**, M. Rezaei-Tavirani, and M. Rostami Nejad, "Comparison of serum zinc concentrations in patients with celiac disease and Crohn's disease in Tehran city", *Scientific Journal of Ilam University of Medical Sciences*.
37. سوئیچ مولکولی آزوینز: یک موتور مولکولی در نانو ماشین های زیستی، فاطمه اکتفا، زهرا اکتفا، فریبا فتحی، ماهنامه فناوری نانو، سال سیزدهم، آبان ماه ۹۳، شماره ۸
38. استفاده از عصاره گیاه میرتکس به عنوان بازدارنده خودگی فولاد در محلول اسید کلریدریک، منصور بزرگ، تقی شهرابی فراهانی، فاطمه اکتفا، فرآیندهای نوین در مهندسی مواد سال ۱۱، شماره ۴، زمستان ۹۶
39. استفاده از عصاره گیاه مورد به عنوان بازدارنده خودگی فولاد در محلول اسید کلریدریک، منصور بزرگ، تقی شهرابی فراهانی، جابر نشاطی، فاطمه اکتفا، فرآیندهای نوین در مهندسی مواد سال ۱۱، شماره ۴، زمستان

❖ Conference Articles

1. **F. Ektefa** and S. Javadian, "Preferential sitting of BEA, FAU, MOR, and MFI zeolite frameworks for adsorbed phenol: A monte carlo study" *5th Iran international zeolite conference, Tabriz, Iran, 26-27 August 2018.*
2. **F. Ektefa** and S. Javadian, "A computational study of the efficiency of nanocrystallin zeolite for separation phenol from water" *6th Theoretical and computational chemistry workshop and seminar, CCER, Tehran, Iran, 1-2 February 2017.*
3. **F. Ektefa**, Y. A. Wang, and S. Javadian, "Temozolomide loading and release from FAU, MOR, LTL, and BEA zeolites as drug delivery systems: A QM/MM computational study", *Medicinal Chemistry, Colby-Sawyer College, New London NH, Massachusetts, United States, 6-7 August 2016.*
4. **F. Ektefa**, Y. A. Wang, and S. Javadian, "A QM/MM computational comparison of efficiency of zeolites as drug delivery systems for temozolomide: host-guest interactions", *21st International Conference on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI), University of British Columbia (UBC), Vancouver, BC, Canada, 2-9 July 2016.*
5. **F. Ektefa**, S. Javadian, and Y. A. Wang, "An efficient approach to explore performance of nanostructure of zeolite: Computational analysis", *10th Annual VIVA NMR Symposium, University of Victoria, Victoria, BC, Canada, 17 June 2016.*
6. **F. Ektefa**, S. Javadian, and Y. A. Wang, *Nanolytica, Simon Fraser University (SFU), Vancouver, BC, Canada, 5 May 2016.*
7. **F. Ektefa**, and S. Javadian, "The adsorption of phenol on the Al-ZSM-5: QTAIM analysis", *Asian Nano forum conference, Kish, Iran, 8-11 March 2015.*
8. **F. Ektefa**, S. Javadian, and S. Soltanali, "A DFT exploration of the adsorption of phenol on the industrial nanostructrured catalyst (ZSM-5)", *2nd International Conference Of Oil, Gas And Petrochemical, Tehran, Iran, 18 December 2014.*
9. **F. Ektefa** and S. Javadian, "DFT Study of Substituted Azobenzene as Corrosion Inhibitors for Mild Steel", *10th Annual Seminar of Electrochemistry of Iran, Tehran, Iran, 26-27 November 2014.*
10. **F. Ektefa**, S. Javadian, and S. Soltanali, "The adsorption of phenol on industrial nanostructured catalyst (ZSM-5): a computational study", *5th International Congress on Nanoscience & Nanotechnology, Tehran, Iran, 22-24 October 2014.*
11. **F. Ektefa**, S. Javadian, and S. Soltanali, "The adsorption of benzene on the industrial catalyst (ZSM-5): a computational study", *17th Conference of Physical Chemistry, Tehran, Iran, 20-22 October 2014.*

12. **F. Ektefa**, M. Anafcheh, and N. L. Hadipour, "An investigation electric field gradient and chemical shielding tensors of azobenzene nanobioswitch: a density functional theory", *3rd International Congress on Nanoscience and Nanotechnology, Shiraz, Iran, 9-11 November 2010.*
13. **F. Ektefa**, M. Anafcheh, and N. L. Hadipour, "Investigation of azobenzene as a nano switch in cyclic peptides: a density function theory study", *6th Annual Seminar of Electrochemistry of Iran, Kish, Iran, 7-10 October 2010.*
14. **F. Ektefa**, M. Anafcheh, and N. L. Hadipour, "Structural study and determination of NQR parameters of azobenzene nanobioswitch using computational chemistry methods", *16th national and 4th international conference of biology, Mashhad, Iran, 14-16 September 2010.*

❖ **Books (in Persian)**

1. Omics: New insight to modern biology, F. Fathi, **F. Ektefa**, and A. Mani, ISBN: 3993357
2. Experiments in physical chemistry, M. Anafcheh, **F. Ektefa**, ISBN: 5032935

✓ **WORKSHOP-----**

1. Workshop on "Molecular dynamic simulation of protein-ligand". *Tarbiat Modares University, Tehran, Iran, Feb 2014.*
2. Workshop on "The modeling and molecular dynamic simulation of nano bio systems by Gromacs Software (1)". *Faculty of Shahid Beheshti Medical Science, Tehran, Iran, June 2012.*
3. Workshop on "The modeling and molecular dynamic simulation of nano bio systems by Gromacs Software (2)". *Faculty of Shahid Beheshti Medical Science, Tehran, Iran, December 2012.*
4. Workshop on "VMD software for simulation results analysis", *Institute for Research in Fundamental Sciences, Tehran, Iran, September 2013.*
5. Workshop on "Molecular dynamic simulation: Lammps", *Amir Kabir University, Tehran, Iran, May 2014.*
6. Workshop on "Molecular dynamic simulation: Material Studio", *Amir Kabir University, Tehran, Iran, May 2014.*
7. Workshop on "Experimental Design", *Iran University of Science and Technology, Tehran, Iran, November 2014.*
8. Workshop on "Computational methods in the electrochemistry", *Iran University of Science and Technology, Tehran, Iran, November 2014.*
9. Workshop on "Method on oral presentation paper", *Tarbiat Modares University, Tehran, Iran, October 2014.*

❖ *Chemometrics, short term training course, winter 2006, Total GPA: 100 (out of 100)*

❖ *Health, Safety and Environment (HSE), training course, winter 2013*

✓ **SKILLS-----**

- ❖ **Language skills**
 - **Persian:** Official language in my country
 - **English:** Intermediate
- ❖ **Software skills:** Gaussian, Gauss View, AIM, Hyperchem, crystal maker, Mercury, Avogadro, Chem Office, Material Studio, VMD, VESTA, DLPOLY, SigmaPlot, Table Curve, MATLAB and Visual FORTRAN (Orientation relative).

- ❖ **Instrumental & Technical Skills:** Sample preparation, Bench Chemistry methods (titration, solvent extraction, etc), UV-Visible Spectroscopy, Atomic Absorption Spectroscopy.
 - ❖ **Other Skills:** Linux, Windows, ICDL, Microsoft Office Package, End note, Photoshop, Research methodology.
- ✓ **EXTRACURRICULAR ACTIVITIES-----**
- ❖ 21st International Conference on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI), University of British Columbia (UBC), Vancouver, Canada (2-9 Jul. 2016)
Member of the Executive Committee
 - ❖ 11th Annual Seminar of Electrochemistry of Iran (18-19 Nov. 2015)
Member of the Executive Committee
 - ❖ 6th Annual Seminar of Electrochemistry of Iran (7-10 Oct. 2010)
Member of the Executive Committee
 - ❖ 5th Annual Seminar of Electrochemistry of Iran (6-7 May 2009)
Member of the Executive Committee
- ✓ **PROFESSIONAL AFFILIATION-----**
- ❖ Iranian Nano Society (2011- present)
 - ❖ Iranian Chemical Society (2011- present)
 - ❖ Iranian Association of Chemical Engineering (2013- present)
 - ❖ Electrochemical Society of Iran (2014- present)
 - ❖ Young researchers and elite club (2015- present)
- ✓ **ACADEMIC REFERENCES-----**
- **Dr. Jafar Towfighi Darian**
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 - **Dr. Naser L. Hadipour**
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 - **Dr. Soheila Javadian Farzaneh**
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 - **Dr. Yan Alexander Wang**
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