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Associate Professor of Physical Chemistry

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Educational Background

- Ph.D. in Physical Chemistry, Sharif University of Technology, Tehran, Iran, 2011.
- M.Sc. in Physical Chemistry, Sharif University of Technology, Tehran, Iran, 2006.
- B.Sc. in Pure Chemistry, Shiraz University, Shiraz, Iran, 2004.

Professional Background

- Assistant Professor of Physical Chemistry, Semnan University, Semnan, Iran, 2011-2020.
- Associate Professor of Physical Chemistry, Semnan University, Semnan, Iran, 2020-present.

Research Interests

- Electrochemical study of anodic and cathodic processes in fuel cells
- Electrochemistry of corrosion and Inhibiting methods of corrosion
- Preparation of micro and nano catalysts by chemical and electrochemical methods and their application as an electrode in anodic and cathodic compartments of fuel cells
- Computational Chemistry

Publications (ISI)

48. Graphene oxide nanosheet as a nanocarrier for the PARP inhibitor NU1025: A DFT and molecular dynamics study, F. Alikhoshi, A. Arab, M. Sadeghi, ***Journal of Molecular Liquids***, 445 (2026) 129213.

47. Computational design of graphene oxide-based delivery of PD128763 PARP inhibitor: DFT, molecular dynamics, and molecular docking analysis, F. Alikhoshi, M. Sadeghi, A. Arab, **Structural Chemistry**, (2026), https://doi.org/10.1007/s11224-025-02692-3.

46. Structural elucidation, DFT and Hirshfeld surface analysis, and molecular docking studies of N2O2-type Schiff base ligands and their Cu (II) and Ni (II) complexes targeting …, M. Behzad, L. Ghasemi, F. Mehraban, A. Abbasi, M. Ashfaq, A. Arab, ***Inorganic Chemistry Communications,*** 182 (2025) 115465.

45. Investigating the possible NU1025 drug delivery with graphene and boron nitride nanosheets using DFT and molecular docking computations, F. Alikhoshi, A. Arab, M. Sadeghi, ***Chemical Physics,*** 595 (2025) 112713.

44. Investigating the corrosion resistance of coated steel with Ni-WP nanocomposites prepared by electroless method, S. Rashid, A. Arab, S. Faraji, ***Applied Chemistry Today***, 20 (74), (2025), 161-174.

43. The inhibitory effect of different surfactants on the corrosion of A335 alloy steel in sodium hydroxide solution, A. Ejlali, A. Arab, ***Applied Chemistry Today***, 20 (75), (2025), 71-82.

42. The performance of PdNi alloy catalysts supported on glassy carbon electrode toward formic acid electro-oxidation, A. Gharib, A. Arab, ***Inorganic Chemistry Communications***, 171 (2025) 113501.

41. Electrochemical Oxidation of Formic Acid on PdM (M=Cr, Mn, Fe, Co, Ni, and Ag) Alloy Nanoparticles with Low M Content: A Comparative Study, A. Gharib, A. Arab, ***ChemistrySelect***, 8 (33), (2023), e202302061.

40. A pyrazolone-based dinuclear Cu (II) Schiff-base complex: DFT studies on the rate-determining steps of the tautomerism in the ligand and molecular docking modelling with COVID …, L. Ghasemi, M. Behzad, A. Gharib, A. Arab, A.R. Abbasi, ***Journal of Coordination Chemistry***, 76 (5-6), (2023), 830-846

39. Decomposition of formic acid via carboxyl mechanism on the graphene nanosheet decorated by Cr, Mn, Fe, Co, Ni, Pd, Ag, and Cd metals: A DFT study, A. Gharib, A. Arab, ***International Journal of Hydrogen Energy***, 48 (2), (2023), 566-575.

38. Comparison of physical/chemical properties of Prussian blue thin films prepared by different pulse and DC electrodeposition methods, V. Bayzi Isfahani, A. Arab, et al., ***Materials***, 15 (24), (2022), 8857

37. Chemically prepared Pd-Cd alloy nanocatalysts as the highly active material for formic acid electrochemical oxidation, A. Gharib, A. Arab, ***Molecular Catalysis***, 528 (2022) 112434.

36. Efficient electrochemical oxidation of reactive dye using a novel Ti/nanoZnO–CuO anode: electrode characterization, modeling, and operational parameters optimization, Nastaran Akbari, Farideh Nabizadeh Chianeh, Ali Arab, ***Journal of Applied Electrochemistry***, 52(1), (2022), 189-202.

35. The inhibition effect of CTAB and Triton X-100 surfactants on the corrosion of nickel in alkaline solution, M. Rajabi, A. Arab, A. Bagheri, ***Applied Chemistry Today***, 16 (59), (2021), 63-72.

34. Synergism of CTAB and NLS surfactants on the corrosion inhibition of mild steel in sodium chloride solution, Bahman Sargolzaei, Ali Arab, ***Materials Today Communications***, 29 (2021) 102809.

33. Gellan-Gum and LiTFSI-Based Solid Polymer Electrolytes for Electrochromic Devices, Vahideh Bayzi Isfahani, Rui FP Pereira, Mariana Fernandes, Rodrigo C Sabadini, Sónia Pereira, Hamid Rezagholipour Dizaji, Ali Arab, Elvira Fortunato, Agnieszka Pawlicka, Rosa Rego, Verónica de Zea Bermudez, Maria M Silva, ***ChemistrySelect,*** 6 (2021) 5110-5119.

32. DFT study of the interaction between carbon monoxide and Rh-Cu bimetallic nanoclusters, Ali Arab, ***Materials Today Communications***, 26 (2021) 102013.

31. Experimentally Designed Natural Light Induced Photocatalytic Performance of Nanostructured Eu2Ce2O7 Synthesized by a Facile Solid State Method in Removal of Environmental Pollutant Malachite

Green (MG), Mina Dolatalizadeh, Mahdi Behzad, Shahin Khademinia, Ali Arab, ***Proceedings of the National Academy of Sciences, India Section A: Physical Sciences***, 91 (2021) 9-20.

30. DFT study of Ni-doped graphene nanosheet as a drug carrier for multiple sclerosis drugs, Najme Dastani, Ali Arab, Heidar Raissi, ***Computational and Theoretical Chemistry***, 1196 (2021) 113114.

29. Improved formic acid oxidation using electrodeposited Pd-Cd electrocatalysts in sulfuric acid solution, Azar Gharib, Ali Arab, ***International Journal of Hydrogen Energy***, 46 (2021) 3865-3875.

28. Systematic Investigation of Structure and Optoelectronic Properties of Gen (n= 3-20), MGe_9 (M= Ga, Si, Sn, As) and $Ga_xGe_{(10-x)}$(x= 1-10) Clusters: Computational Approach, Zabiollah Mahdavifar, Mina Afshari, Ahmad Bagheri, Ali Arab, ***Polyhedron***, 193 (2021) 114874.

27**.** Enhanced Electrocatalytic Activity of Low Ni Content Nano Structured NiPd Electrocatalysts Prepared by Electrodeposition Method for Borohydride Oxidation, Mahdieh Zolfaghari, Ali Arab, Alireza Asghari, ***Journal of Electrochemical Science and Technology***, 11 (2020) 238-247.

26. DFT computational study towards investigating Cladribine anticancer drug adsorption on the graphene and functionalized graphene, Najme Dastani, Ali Arab, Heidar Raissi, ***Structural Chemistry,*** 31 (2020) 1691-1705.

25. Biginelli reaction catalyzed by elemental bromine as a novel Lewis acid catalyst, under mild conditions, M. Robati E. Kolvari, A. Arab, ***Eurasian Chemical Communications***, 2 (2020) 909-915.

24. Adsorption of Ampyra anticancer drug on the graphene and functionalized graphene as template materials with high efficient carrier, Najme Dastani, Ali Arab, Heidar Raissi, ***Adsorption,*** 26 (2020) 879–893.

23. Electrodeposited Pd, PdCd, and PdBi nanostructures: Preparation, characterization, corrosion behavior, and their electrocatalytic activities for formic acid oxidation, Azar Gharib, Ali Arab, ***Journal of Electroanalytical Chemistry***, 866 (2020) 114166.

22. Electrodeposition of prussian blue films: study of deposition time effect on electrochemical properties, Vahideh Bayzi Isfahani, Hamid Rezagholipour Dizaji, Nafiseh Memarian, Ali Arab, ***Materials Research express***, 6 (2019) 096449.

21. The formate and redox mechanisms of water-gas shift reaction on the surface of Ag: A nanocluster model based on DFT study, Darioush Sharafie, Ali Arab, Mostafa Fazli, ***Iranian Journal of Catalysis,*** 9(3) (2019) 213-221.

20. Surfactant-Assisted Electrodeposition of Nickel Nanostructures and Their Electrocatalytic Activities Toward Oxidation of Sodium Borohydride, Ethanol, and Methanol, Mahdieh Zolfaghari, Ali Arab, Alireza Asghari, ***ChemistrySelect***, 4(2019) 4487–4495.

19. The physical and electrochromic properties of Prussian Blue thin films electrodeposited on ITO electrodes, V. Bayzi Isfahani, N. Memarian, Hamid Rezagholipour Dizaji, A. Arab, M.M. Silva, ***Electrochimica Acta***, 304 (2019) 282-291.

18. New copper(II) and vanadium(IV) complexes based on allylaminederived Schiff base ligand; synthesis, crystal structure, electrochemical properties and DFT calculations, Armaghan Behnam Deilami , Mehdi Salehi, Ahmad Amiri , Ali Arab, ***Journal of Molecular Structure,*** 1181 (2019) 190-196.

17. Synthesis, crystal structure, electrochemical properties and DFT calculations of three new Zn(II), Ni(II) and Co(III) complexes based on 5-bromo-2-((allylimino)methyl)phenol Schiff-based ligand, Armaghan Behnam Deilami , Mehdi Salehi, Ali Arab, Ahmad Amiri, ***Inorganica Chimica Acta,*** 476 (2018) 93–100.

16. Crystal structures, DFT calculations, and Hirshfeld surface analyses of two new copper(II) and nickel(II) Schiff base complexes derived from meso-1,2-diphenyl-1,2-ethylenediamine, Leila Seifikar Ghomi, Mahdi Behzad, Atekeh Tarahhomi, Ali Arab, ***Journal of Molecular Structure,*** 1150 (2017) 214-226.

15. Theoretical study of water-gas shift reaction on the silver nanocluster, Ali Arab, Darioush Sharafie, Mostafa Fazli, ***Journal of Physics and Chemistry of Solids,*** 109 (2017) 100–108.

14. DFT studies and antioxidant activity of Schiff base metal complexes of 2-aminopyridine. Crystal structures of cobalt(II) and zinc(II) complexes, Mahbobeh Jafari, Mehdi Salehi, Maciej Kubicki, Ali Arab, Ali Khaleghian, ***Inorganica Chimica Acta,*** 462 (2017) 329–335.

13. DFT study of nitrogen monoxide adsorption and dissociation on Rh-Cu nano clusters, A. Arab, M. Nahali, F. Gobal, ***Journal of Alloys and Compounds,*** 695 (2017) 1924-1929.

12. Crystal structures, DFT calculations and Hirshfeld surface analyses of three new cobalt(III) Schiff base complexes derived from meso-1,2-diphenyl-1,2-ethylenediamine, Mohaddeseh Masoudi, Mahdi Behzad, Ali Arab, Atekeh Tarahhomi, Hadi Amiri Rudbari, Giuseppe Bruno, ***Journal of Molecular Structure,*** 1122 (2016) 123-133.

11. Electronic structure and reactivity of $(TiO2)_n$ (n=1–10) nano-clusters: Global and local hardness based DFT study, Ali Arab, Fatemeh Ziari, Mostafa Fazli, ***Computational Materials Science,*** 117 (2016) 90–97.

10. Catalytic behavior of an iron(III) complex containing an N,O-type bidentate oxazoline ligand for selective oxidation of sulfides, Mojtaba Amini, Mostafa Khaksar, Ali Arab, Reza Masoomi Jahandizi, Mojtaba Bagherzadeh, Davar M. Boghaei, Arkady Ellern, L. Keith Woo, ***Transition Metal Chemistry*****,** 41(2016) 97–105.

9. Synthesis, structure, and catalytic properties of copper, palladium and cobalt complexes containing an N,O-type bidentate thiazoline ligand, Mojtaba Amini, Arshad Bayrami, Mohammad Nazari Marashi, Ali Arab, Arkady Ellern, L. Keith Woo, ***Inorganica Chimica Acta*****,** 443 (2016) 22–27.

8. Comparative hydrogen adsorption on the pure Al and mixed Al-Si nano clusters: A first principle DFT study, A. Arab, M. Habibzadeh, ***Computational and Theoretical Chemistry***, 1068 (2015) 52–56.

7. A novel iron complex containing an N,O-type bidentate oxazoline ligand: Synthesis, X-ray studies, DFT calculations and catalytic activity, M. Amini, A. Arab, P. Gohari Derakhshandeh, M. Bagherzadeh, A. Ellern, L. K. Woo, ***Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*****,** 133 (2014) 432–438.

6. Synthesis, X-ray structure, DFT studies, and catalytic activity of a vanadium(V) complex containing a tridentate Schiff base, M. Amini, A. Arab, R. Soleyman, A. Ellern, L. K. Woo, ***Journal of Coordination Chemistry***, 66 (2013) 3770–3781.

5. Electronic and Structural Properties of Neutral, Anionic, and Cationic Rh_xCu_{4-x} (x=0-4) Small Clusters: A DFT Study, A. Arab, F. Gobal, N. Nahali, M. Nahali, ***Journal of Cluster Science***, 24 (2013) 273-287.

4. Adsorption and dissociation of hydrogen peroxide on small Pd_xM_{3-x} (M=Pt, Cu;x=1-3) clusters: a hybrid density functional study, F. Gobal, M.Nahali, R. Arab, ***Molecular Physics***, 109 (2011) 1797-1804.

3. Electro-deposited Rh and Rh-Cu alloys as ethanol tolerant electro-catalysts for oxygen reduction in alkaline media, F. Gobal, R. Arab, ***Electrocatalysis***, 2 (2011) 42-51.

2. A comparative study of atomic and molecular oxygen adsorption on neutral and negatively charged Pd_xCu_{3-x} (x=0-3) nano-clusters, F. Gobal, R. Arab, M. Nahali, ***J. Mol. Structure (THEOCHEM)*** 959 (2010) 15-21.

1. A preliminary study of the electro-catalytic reduction of oxygen on Cu-Pd alloys in alkaline solution, F. Gobal, R. Arab, ***J. Electroanal. Chem.***, 647 (2010) 66-73.

Publications (ISC)

9. اثر بازدارندگی سورفکتانت های تریتون X-100 و CTAB بر خوردگی نیکل در محلول قلیایی، مژگان رجبی، علی عرب، احمد باقری، **مجله علمی- پژوهشی شیمی کاربردی** سال شانزدهم، شماره 59 تابستان1400، صفحه 63.

8. Interaction and micellar behavior of aqueous mixtures of surface active ionic liquid and cationic surfactant: experimental and theoretical studies, Niloofar Faraji, Ahmad Bagheri, Ali Arab, ***Journal of Applied Chemistry***, 14(53) (2020) 43-54.

7. بررسی جذب نیتروژن مونو اکسید روی نانو کلاسترهای Rh-Cu نشانده شده بر بستر نانو صفحه گرافن با استفاده از نظریه تابعی دانسیته، آرزو قاسمی، علی عرب، **نشریه علمی- پژوهشی نانومقیاس**، سال پنجم، شماره چهارم، زمستان 97، صفحه 305.

6. On the morphology and corrosion behavior of Ni nanostructures electrodeposited in the presence of different surfactants, Mahdieh Zolfaghari, Ali Arab, ***Journal of Applied Chemistry,*** 13 (2019) 45-52.

5. مطالعه خواص ساختاری و الکترونی نانوکلاسترهای نقره (Ag_2-Ag_{10}) *و بررسی* برهمکنش آن ها با کربن مونو اکسید به روش نظریه تابعی دانسیته، داریوش شرفی، علی عرب، مصطفی فضلی، **مجله علمی- پژوهشی شیمی کاربردی** سال سیزدهم، شماره 46 بهار 1397، صفحه 171.

4. Theoretical Study of OH Adsorption on Pd_xCu_{3-x} (x = 0-3) Nano Clusters, Ali Arab, Fereydoon Gobal, ***International Journal of Nanoscience and Nanotechnology***, 13 (2017) 299-306.

3. Theoretical study of geometry, stability and properties of Al and AlSi nano clusters, Ali Arab, Mohaddeseh Habibzadeh, **Journal of Nanostructure in Chemistry,** 6 (2016) 111–119.

2. مطالعه نظری جذب اکسیژن روی نانوکلاسترهای خالص و ترکیبی Rh وCu ، علی عرب، فریدون گبل، **مجله علمی- پژوهشی شیمی کاربردی** سال دهم، شماره 34 بهار 1394، صفحه 35.

1. On the catalytic behavior of copper toward oxygen reduction reaction in alkaline solution, A. Arab, F. Gobal, ***Journal of Applied Chemistry,*** 7 (2013) 23-30.

Conference Papers

18. اثر بازدارندگی سورفکتانت های مختلف روی خوردگی فولاد آلیاژی A335درمحلول سدیم هیدروکسید. عباس اجلالی، علی عرب، هفتمین کنفرانس شیمی کاربردی انجمن شیمی ایران (1403).

17. تهیه پوشش های نانوکامپوزیتی Ni-Co-P وNi-Co-P-SiC به روش الکترولس جهت ممانعت از خوردگی فولاد، الهه کیقبادی، علی عرب، سهیلا فرجی، هفتمین کنفرانس شیمی کاربردی انجمن شیمی ایران (1403).

16. مطالعات اتصال مولکولی مهارکنندههای (PARP-1 Poly (ADP-ribose) polymerase-1) با مطالعه داکینگ مولکولی، فهیمه علی خوشی، علی عرب، مهدی صادقی، بیست و سومین کنگره ملی و یازدهمین کنگره بین المللی زیست شناسی ایران، (1403).

15. The corrosion behaviour of electrodeposited Pd, Pd-Cd, and Pd-Bi samples in sulphuric acid solution: An electrochemical study, Azar Gharib, Ali Arab, **26th Iranian Conference of Analytical Chemistry**, Semnan, Iran, 2019.

14. The inhibition effect of CTAB surfactant on the corrosion of mild steel in 3.5% NaCl solution, Bahman Sargolzaei, Ali Arab, **26th Iranian Conference of Analytical Chemistry**, Semnan, Iran, 2019.

13. Electro-oxidation of ethanol on the nanostructured bimetallic NiPd electrocatalysts in alkaline solution, Mahdieh Zolfaghari, Ali Arab, Alireza Asghari, **26th Iranian Conference of Analytical Chemistry**, Semnan, Iran, 2019.

12. حذف رنگزای راکتیو نارنجی 7 با استفاده از نانو کامپوزیتZnO-CuO ، نسترن اکبری، فریده نبی زاده چیانه، علی عرب، **چهارمین کنفرانس شیمی کاربردی ایران**، ارومیه، ایران، مرداد ۱۳۹۸.

11. Molecular structure and electronic properties of adsorbed Ampyra drug on the functionalized graphene nanosheet: A DFT study, Najme Dastani, Ali Arab, Heidar Raissi, **The 20th Iranian Chemistry Congress**, Mashhad, Iran, 2018.

10. Density functional calculations on the adsorption of Ampyra drug on graphene nanosheet, Najme Dastani, Ali Arab, Heidar Raissi, **The 20th Iranian Chemistry Congress**, Mashhad, Iran, 2018.

9. Effect of surfactant and electrodeposition method on the structure and morphology of nickel electrodeposits, Mahdieh Zolfaghari, Ali Arab, **19th Iranian Physical Chemistry Conference**, Zibakenar, Iran, (2016).

8. Protection of Copper, Brass and Steel in glycolic solution using different inhibitors, Niusha Zolfaghari, Ali Arab, **19th Iranian Physical Chemistry Conference**, Zibakenar, Iran, (2016).

7. Theoretical study of reactivity of each atom in $(TiO_2)_n$ (n=1-5) nano-clusters on the basis of local hardness**,** Fatemeh Ziari, Ali Arab, **The 18th Iranian Chemistry Congress**, Semnan, Iran, (2015).

6. DFT study of structure and stability of Cu_n(n=1-10) nano clusters, Hajar Jafarinia, Ali Arab, **The 18th Iranian Chemistry Congress**, Semnan, Iran, (2015).

5. On the geometries and electronic properties of (TiO_2)n (n=1-5) nano-clusters: A DFT study, Fatemeh Ziari, Ali Arab, **The 18th Iranian Chemistry Congress**, Semnan, Iran, (2015).

4. Investigation of electronic structure and geometry of silver nano clusters using density functional theory, Darioush Sharafie, Ali Arab, **The 18th Iranian Chemistry Congress**, Semnan, Iran, (2015).

3. Electronic Structure and Properties of Al Nano-Clusters as a Function of Size: A DFT Study, *M. Habibzadeh, A. Arab,* **17th Iranian Physical Chemistry Conference**, Tehran, Iran, (2014).

2. Effect of copper oxide formation on the kinetics and mechanism of oxygen reduction reaction on copper, A. Arab, F. Gobal, **15th Iranian Physical Chemistry Conference**, Tehran, Iran, (2012).

1. Effect of Cu insertion on the structure and electronic properties of small Rh clusters: A DFT study, A. Arab, F. Gobal, M. Nahali, **15th Iranian Physical Chemistry Conference**, Tehran, Iran, (2012).

Courses Taught

1-General Chemistry (I&II) (undergraduate)

2- Physical Chemistry (I&II) (undergraduate)

3-Corrosion of Metals (undergraduate)

4- Quantum Chemistry (undergraduate)

5- Advanced Physical Chemistry (graduate, MSc)

6-Advanced Electrochemistry (graduate, MSc)

7- Statistical Thermodynamic (graduate, MSc)

8- New Topics in Electrochemistry (graduate, PhD)

9- New Topics in Physical Chemistry (graduate, PhD)

Ph.D. Thesis Supervised

5. Fahime Alikhoshi, **Investigating the interaction between poly ADP Ribose polymerase (PARP) inhibitors and modified graphene nanosheet using quantum computations, molecular docking, and molecular dynamics simulation**, Department of Chemistry, Semnan University, 2025.

4. Azar Gharib, **Preparation and characterization of glassy carbon electrode modified with metal nano-particles for formic acid oxidation and theoretical study of the adsorption and dissociation of formic acid on the graphene nano sheets modified with these metals**, Department of Chemistry, Semnan University, 2022.

3. Najme Dastani, **Investigation of the interaction between MS drugs and modified graphene nanosheets for use in drug delivery systems**, Department of Chemistry, Semnan University, 2021.

2. Mahdieh Zolfaghari, **Electro-Oxidation of Sodium Borohydride and Alcohols on Nanostructured Ni and Ni-Alloys Electro-Catalysts for Application in Fuel Cells,** Department of Chemistry, Semnan University, 2019.

1. Darioush Sharafie, **Theoretical Study of Kinetics of Water – Gas Shift Reaction on the Silver Nanoclusters Supported on the Graphene Nanosheets,** Department of Chemistry, Semnan University, 2017.

M.Sc. Thesis Supervised

18. Sakine Khademian, **Electrochemical study of the inhibition effect of surfactants in the presence of graphene oxide on the corrosion of steel in hydrochloric acid solution**, Department of Chemistry, Semnan University, 2023.

17. Zhila Valizade, **Adsorption of Thiotepa anticancer drug on the single-walled carbon nanotube using density functional theory**, Department of Chemistry, Semnan University, 2023.

16. Abbas Ejlali, **The study of the inhibition effect of SDS and DOTAB surface active agents on the corrosion of A335 steel in sodium hydroxide solution**, Department of Chemistry, Semnan University, 2022.

15. Hadiye Arabameri, **Theoretical study of the structural and electronic properties of ionic liquids consist of 1-ethyl-3-methyl-imidazolium cation with different anions**, Department of Chemistry, Semnan University, 2021.

14. Sima Rashid, **Preparation of Ni-W-P nanocomposite coatings in the presence of SiC nano-particles by electroless plating on the mild steel and investigation of their corrosion and hardness behaviors**, Department of Chemistry, Semnan University, 2021.

13. Mohadese Fathalizade, **Theoretical study of the structural and electronic properties of ionic liquids consist of 1, 2, 4-Triazolium cation with different anions**, Department of Chemistry, Semnan University, 2021.

12. Mohammad Amin Jamali, **Electrochemical study of the inhibition effect of CTAB and NLS surfactants on the corrosion of steel in hydrochloric acid solution**, Department of Chemistry, Semnan University, 2021.

11. Elahe Keyghobadi, **Preparation of Ni-Co-P nanocomposite coatings in the presence of SiC nano-particles by electroless plating on the mild steel and investigation of their corrosion and hardness behaviors**, Department of Chemistry, Semnan University, 2021.

10. Naser Abniki, **The Study of CO Adsorption on the Graphene Nano-sheets Modified with Transition Metals Using Quantum Computations**, Department of Chemistry, Semnan University, 2021.

9. Bahman Sargolzaei, **Study of Surfactants Inhibition Effect on the Corrosion of Steel by Electrochemical Methods in Sodium Chloride Solution,** Department of Chemistry, Semnan University, 2020.

8. Mojgan Rajabi, **The performance of surfactants as corrosion inhibitors for Nickel in alkaline solution,** Department of Chemistry, Semnan University, 2019.

7. Aliyeh Hematian, **Theoretical study of the structural and electronic properties of some ammonium-based ionic liquids,** Department of Chemistry, Semnan University, 2019.

6. Arezoo Ghasemi, **Theoretical study of nitrogen monoxide adsorption on the Rh-Cu nano-clusters supported on graphene nano sheets**, Department of Chemistry, Semnan University, 2017.

5. Mohammad Karaimi, **Electrodeposition and corrosion study of Ni nanostructures in acidic solution**, Department of Chemistry, Semnan University, 2017.

4. Niusha Zolfaghari, **The study of anti-corrosion behavior of Benzotriazole and benzothiazole derivatives for the copper, brass, aluminum, steel, cast iron and solder metals in glycol antifreeze**, Department of Chemistry, Semnan University, 2017.

3. Hajar Jafarinia, **A theoretical study of the interaction between Cu nanoclusters and some diatomic molecules such as NO and CO on the basis of chemical hardness**, Department of Chemistry, Semnan University, 2015.

2. Fatemeh Ziari, **Theoretical study of pure and rare earth metal doped TiO_2 nanoclusters**, Department of Chemistry, Semnan University, 2015.

1. Mohaddeseh Habibzadeh, **Theoretical study of hydrogen adsorption on Al and AlSi nanoclusters**, Department of Chemistry, Semnan University, 2014.