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

Publications (ISI)

35. 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***, (2021). https://doi.org/10.1007/s10800-021-01634-1.

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)

۹. 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 ۵۹ تابستان ۱۴۰۰، صفحه ۶۳.

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.

۷. 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 ۹۷، صفحه ۳۰۵.

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 ۴۶ بهار ۱۳۹۷، صفحه ۱۷۱.

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 ۳۴ بهار ۱۳۹۴، صفحه ۳۵.

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

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.

۱۲. 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

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

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.