Ali Arab

Assistant 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-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)

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)

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

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 (I) (graduate, MSc)

8- Applied Electrochemistry (graduate, PhD)

9- New Topics in Electrochemistry (graduate, PhD)

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

MSc Thesis Supervised

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.