



Ali Arab

Assistant Professor of Physical Chemistry
Department of Chemistry, Semnan University
Semnan, Iran

Email: a.arab@semnan.ac.ir

aliarab.su@gmail.com

Tel: +98-23-33383195

Fax: +98-23-33654110

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)

11. Electronic structure and reactivity of $(\text{TiO}_2)_n$ ($n=1-10$) 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**, 2016, DOI :10.1007/s40097-015-0185-7.

2. مطالعه نظری جذب اکسیژن روی نانوکلاسترهای خالص و ترکیبی Cu و Rh ، 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

7. Theoretical study of reactivity of each atom in $(\text{TiO}_2)_n$ ($n=1-5$) 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 $(\text{TiO}_2)_n$ ($n=1-5$) 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)