Curriculum Vitae

Dr. Razieh Habibpour Gharacheh

Assistance Professor in Physical Chemistry

Permanent Address

Department of Catalysis & Inorganic Chemical Technology, Institute of Chemical Technology, Iranian Research Organization for Science and Technology (IROST),

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Education

1) Ph. D, In Physical Chemistry, University of Isfahan, Isfahan, Iran (2013).

Thesis Title: Study of Au nano-catalysts electronic properties and effect of Pt, Cu, and Fe metals on their catalytic activity using quantum mechanics methods.

3) M. Sc, In Physical Chemistry, Sistan and Baluchestan University, Zahedan, Iran (2005).

Thesis Title: Effects of different supports and promoters on the morphology and function of mixed iron-cobalt oxide catalysts for the conversion of synthesis gas to light olefins.

4) B. Sc, In Chemistry, Shahid Bahonar University, Kerman, Iran (2001).

Research interest

1) Fischer-Tropsch synthesis (catalysts preparation and performance evaluation)

2) Design (computational modeling) of catalysts and new materials.

3) Quantum mechanics calculations (ab initio, semi-empirical and density-functional theory) to solve problems in chemistry.

4) Computational design of drugs

5) Solvent Extraction

Research Pojects

1) Preparation of effective and sustainable catalysts for conversion of synthesis gas to ethylene and propylene

2) Identification of rare-earths elements (REEs) found in the Angouran mine ore in various mineral zones and the extraction of these elements.

3) Stripping Rare Earth Elements and Iron from D2EHPA as Organic Extractant and Kerosene as Diluent during Zinc Solvent Extraction

4) Design and evaluate new multifunctional ligands as effective compounds to treat Alzheimer's disease using computational methods

5) Scandium oxide extraction from waste produced by Alumina Company of Iran.

Skills

Trained with: XRD, XRF, GC, and BET.
Familiar with: Linux, Quantum Espresso, Crystal Maker, Nanotube Modeler, Gauss View, GaussSum, Gaussian, and Gromacs.

Supervisor of 6 master's theses and 1 Ph.D. Thesis

1) **Title:** Study of the electronic properties and structural stability of cadmium oxide nano-clusters using density functional theory, **Student:** Mousa Asadi

2) **Title:** Investigation of the effect of oxygen adsorption on the stability and electronic properties of $Sn_mGe_n(m+n\leq4)$ Nano-clusters by density functional theory method, **Student:** Mina Toufanian

3) **Title:** Investigation of H_2O adsorption on Zn_mO_n (m + n =2-4) nanoclusters using DFT, **Student:** Elham Khalese

4) **Title:** Investigation of the thermodynamic and mechanism of the solvent extraction of the lighter lanthanide metal ions by means of organophosphorus extractants: D2EPHA, PC88A, CYANEX272, CYANEX301, **Student:** Maryam Bagherpour

5) **Title:** Theoretical investigation of NO_x detection by Graphene-Boron Nitrid Hybrid Nanoribbons, **Student:** Sotoudeh Delavarkhan

6) **Title:** Computational investigation of edge halogenation of hybrid graphene-boron nitride nanoribbons and study of ripple edge effects on their stability, structural, electronic and chemical properties, **Student:** Zahra Soltani

7) **Title:** Simulation of dens gas dispersion in the dusty environment, **Student:** Narjes Hemmati

Publications

a. Papers:

1) A. A. Mirzaei, R. Habibpour and E. Kashi, "Preparation and optimization of mixed iron cobalt oxide catalysts for conversion of synthesis gas to light olefins" **Applied Catalysis A: General** 296 (2005) 222–23.

2) A. A. Mirzaei, R. Habibpour, E. Kashi, M. Feizi, "Characterization of iron-cobalt oxide catalysts: effect of different supports and promoters upon the structure and morphology of precursors and catalysts" **Applied Catalysis A: General** 301 (2006) 272–283.

3) A. A. Mirzaei, M. Faizi, R. Habibpour, "Effect of preparation conditions on the catalytic performance of cobalt manganese oxide catalysts for conversion of synthesis gas to light olefins" **Applied Catalysis A: General** 306 (2006) 98–107.

4) S. Jalili, A. Zeini Isfahani, R. Habibpour, "Atomic oxygen adsorption on Au (100) and bimetallic Au/M (M = Pt and Cu) surfaces" **Computational and Theoretical Chemistry**, 989 (2012) 18.

5) S. Jalili, A. Zeini Isfahani, R. Habibpour, "DFT Investigations on the Interaction of Oxygen Reduction Reaction Intermediates with Au (100) and Bimetallic Au/M (100) (M = Pt, Cu and Fe) Surfaces" **International Journal of Industrial Chemistry** 4 (2013) 33.

6) R. Habibpour, R. Vaziri, "Computational study of electronic, spectroscopic, and chemical properties of $(CdO)_n$ (n=1-7) nanoclusters as a transparent conducting oxide" **Journal of Particle Science & Technology**, 1 (2015) 195-204.

7) R. Habibpour, R. Vaziri, **"**Computational and theoretical study of electronic, spectroscopic and chemical properties of $(ZnO)_n$ ($n\leq4$) nanoclusters**" Journal of Research on Many-body Systems**, (2015).

8) R. Habibpour, R. Vaziri, "Investigation of structural and electronic properties of small Au_nCu_m ($n+m\leq5$) nano-clusters for oxygen adsorption" **International Journal of Nano Dimension**, 7 (2016) 208-224.

9) R. Habibpour, M. Dargahi, M. Bagherpour, E. Kashi, "Comparative study on Ce (III) and La (III) solvent extraction and separation from a nitric acid medium by D2EHPA and Cyanex272" **Metallurgical Research & Technology**, DOI: 10.1051/metal/2017083.

10) E. Kashi, R. Habibpour, A. Maleki, H. Gorzin, "Effective parameters interaction study in cerium extraction from sulfuric media using di-(2-ethylhexyl) phosphoric acid" **Chemistry & Chemical Technology**, 11 (2017) 144-151.

11) R. Habibpour, E. Kashi, R. Vaziri, "Computational Study of Electronic, Spectroscopic, and Chemical Properties of Cu_n(n=2-8) nanoclusters for CO Adsorption" **International Journal of Nano Dimension**, 8 (2017) 114-123.

12) Razieh Habibpour, Eslam Kashi, "Interaction of atomic hydrogen with monometallic Au(100), Cu(100), Pt(100) surfaces and surface of bimetallic Au@Cu(100), Au@Pt(100) overlayer systems: The role of magnetism" **Iranian Journal of Hydrogen & Fuel Cell**, 3(2017) 209-218.

13) R. Habibpour, E. Kashi, R. Vazirib, "N-doped Hybrid Graphene and Boron Nitride Armchair Nanoribbons as Nonmagnetic Semiconductors with Widely Tunable Electronic Properties" **Russian Journal of Physical Chemistry A**, 92 (2018) 530-537.

14) Eslam Kashi, Razieh Habibpour, Hesamoddin Gorzin, Armin Maleki, "Solvent Extraction and Separation of Light Rare Earth Elements (La, Pr and Nd) in the Presence of Lactic Acid as a Complexing Agent by Cyanex 272 in Kerosene and the Effect of Citric Acid, Acetic Acid and Titriplex III as Auxiliary Agents" **Journal of Rare Earths**, 36 (2018) 317-323.

b. Conference papers

1) 1. A. A. Mirzaei, M. Habibi, R. Habibpour, "**Effect of Preparation Condition on the Catalytic Performance of Iron-Cobalt Oxide atalysts for the Hydrogenation of Carbon Monoxide to Light Olefins**" 8th Iranian inorganic chemistry conference, azarbaijan university of tarbiat moallem, 2004.

2) A. A. Mirzaei, M. Habibi, R. Habibpour, "**Effect of Promoter and Support Loadingon on Activity and Selectivity of Iron-Cobalt Oxide Catalysts**" 8th Iranian inorganic chemistry conference, Azarbaijan university of tarbiat moallem, 2004.

3) A. A. Mirzaei, M. Habibi, R. Habibpour, "**Performance of Fe-Co Supported and promoted Catalysts for directly Producing Light Olefins via Hydrogenation of Carbon Monoxide**" 7th conference of physical chemistry, Esfahan university of technology, 2005.

4) S. Jalili, A. Zeini Isfahani, R. Habibpour, "**Role of Strain and Ligand Effects in the Modification of the Electronic and Chemical Properties of Au/M (M=Pt, Cu and Fe) Bimetallic Surfaces**" 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.

5) S. Jalili, A. Zeini Isfahani, R. Habibpour, "**Effects of Electronic Structure Modifications on the Adsorption of Oxygen Reduction Reaction Intermediates on Au(100)/M (M=Pt, Cu and Fe) surfaces**" 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.

6) S. Jalili, A. Zeini Isfahani, R. Habibpour, "**Atomic Oxygen Adsorption on Au(100) and Au/M (M = Pt, Cu and Fe) Bimetallic Surfaces: Effects of Coverage**" 14th Iranian Physical Chemistry Conference, University of Tehran, Kish, February 25-28, 2011.

7) S. Jalili, A. Zeini Isfahani, R. Habibpour, "**Study of Au Nanocatalysts, Electronic Properties and Effect of Pt, Cu and Fe metals on Their Catalytic Activity Using Density Functional Theory** " 16th Iranian Physical Chemistry Conference, University of Mazandaran, Babolsar, October 28-30, 2013.

8) R. Habibpour, R. Vaziri, "**Superconductivity of Nitrogen Doped Graphite Intercalated with La and Ce**" 17th Iranian Chemical Conference, Vali-e-Asr University of Rafsanjan, Rafsanjan, September 1, 2014.

9) R. Habibpour, R. Vaziri, "**Application of Nitrogen Doped Graphite Intercalated Compounds NdC6 and PrC6 in Batteries**" 17th Iranian Chemical Conference, Vali-e-Asr University of Rafsanjan, Rafsanjan, September 1, 2014.

10) M. Bagherpour, R. Habibpour, M. Dargahi, "**Thermodynamic and mechanism of the solvent extraction of the La3+ metal ion by means of Di-(2-Ethylhexyl)phosphoric acid and Bis(2,4,4-trimethylpentyl) phosphinic acid extractants**" 18th Iranian Chemistry Congress, University of Semnan, Semnan, August 30 – September 1, 2015.

11) R. Habibpour, R. Vaziri, "**Engineering the Work Function and Electronic Emission of Hybrid Graphene-Boron Nitride Armchair Nanoribbon using B-doping"** 19th Iranian Physical Chemistry Conference, University of Guilan, Rasht, September 13-15, 2016.

12) R. Habibpour, R. Vaziri, "**Lithium Adsorption on Armchair Graphene Nanoribbon: Insight from Theory"** 19th Iranian Physical Chemistry Conference, University of Guilan, Rasht, September 13-15, 2016.

13) R. Habibpour, "**Sodium Adsorption on Boron Nitride Armchair Nanoribbon: Insight from DFT**" 20th Iranian Physical Chemistry Conference, University of Arak, Arak, August 20-22, 2017.

14) R. Habibpour, "**Atomic Scale Investigation of nitrogen doping effects on the structural and electronic properties of Boron Nitride Embedded Armchair Graphene Nanoribbons**" 20th Iranian Physical Chemistry Conference, University of Arak, Arak, August 20-22, 2017.

15) R. Habibpour, E. Kashi, "**Evaluation of the selectivity on the La(III)/Ce(III) separation from nitric acid medium with D2EHPA and Cyanex272 extractants**" 25th Iranian Organic Chemistry Conference, Iran University of Science and Technology, Tehran, September 2-4, 2017.

16) R. Habibpour, E. Kashi, "**Study of the F-terminated Boron Nitride Armchair Nanoribbon**" 25th Iranian Organic Chemistry Conference, Iran University of Science and Technology, Tehran, September 2-4, 2017.

Courses taught

1) Physical Chemistry I, BSc level.

2) Physical Chemistry II, BSc level.

3) General Chemistry, BSc level.

4) Physical Chemistry Labs: I and II, BSc level.

5) Elementary Quantum Chemistry, BSc level.

6) Theoretical Chemistry of Nanostructures, MSc level.

7) Computational Chemistry, MSc level

8) Molecular Spectroscopy, MSc level

8) Safety in the Process Industries, PhD level