Ebrahim Ghasemy

♂ Date of Birth: 14/10/1990

PhD Student in Energy and Materials Science

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Education

- PhD Student in Energy and Materials Science
  Énergie Matériaux Télécommunications (EMT) Research Centre at Institut National de la Recherché Scientifique (INRS), Varennes, Canada, Started on Jan. 2021
  Supervisors: Prof. Kulbir Kaur Ghuman and Prof. Ana C. Tavares

- M.Sc. in Materials Engineering, Discipline: Nanotechnology
  Iran University of Science and Technology (IUST), Iran, Dec. 2016
  Supervisors: Prof. Alimorad Rashidi, and Dr. Hosein Banna Motejadded (Advisor: Dr. Tayebeh Hamzehlouyan)
  GPA: 3.81/4

- B.Sc. in Materials Engineering, Discipline Industrial Metallurgy
  University of Maragheh, Iran, Sep. 2013
  Supervisor: Dr. Behnam Seyyedi
  GPA: 3.13/4 (last two years: 3.43/4)

Publications

Journals:

1. **Ghasemy, E.**, Miri Jahromi, A., Khedri, M., Zandi, P., Maleki, R., & Tayebi, L. **(2021)**. In-silico study on viability of MXenes in suppressing the coronavirus infection and distribution. ***Journal of Biomolecular Structure and Dynamics***, 1-7.

2. Khedri, M., Maleki, R., Khiavi, S. G., Ghasemi, M., **Ghasemy, E**., Jahromi, A. M., & Razmjou, A. **(2021)**. Removal of phenazopyridine as a pharmacological contaminant using nanoporous metal/covalent-organic frameworks (MOF/COF) adsorbent. ***Applied Materials Today***, *25*, 101196.

3. Meshkat, S. S., **Ghasemy, E**., Rashidi, A., Tavakoli, O., & Esrafili, M. **(2021)**. Experimental and DFT insights into nitrogen and sulfur co-doped carbon nanotubes for effective desulfurization of liquid phases: Equilibrium & kinetic study. ***Frontiers of Environmental Science & Engineering***, *15*(5), 1-14.

4. Zandi, P., **Ghasemy, E**., Khedri, M., Rashidi, A., Maleki, R., & Miri Jahromi, A. **(2021)**. Shedding light on miniaturized dialysis using MXene 2D materials: A computational chemistry approach. ***ACS omega,*** *6*(9), 6312-6325.

5. Alivand, M. S., Tehrani, N. H. M. H., Askarieh, M., **Ghasemy, E.**, Esrafili, M. D., Ahmadi, R., ... & Rashidi, A. **(2021)**. Defect engineering-induced porosity in graphene quantum dots embedded metal-organic frameworks for enhanced benzene and toluene adsorption. ***Journal of Hazardous Materials***, *416*, 125973.

6. Ettefaghi, E., Rashidi, A., Ghobadian, B., Najafi, G., **Ghasemy, E**., Khoshtaghaza, M. H., ... & Mazlan, M. **(2021)**. Bio-nano emulsion fuel based on graphene quantum dot nanoparticles for reducing energy consumption and pollutants emission. ***Energy***, *218*, 119551.

7. Daraee, M., Saeedirad, R., **Ghasemy, E**., & Rashidi, A. **(2021)**. N-CNT/ZIF-8 nano-adsorbent for adsorptive desulfurization of the liquid streams. ***Journal of Environmental Chemical Engineering***, *9*(1), 104806.

8. Fakhraie, S., Rajabi, H. R., Rashidi, A., Orooji, Y., **Ghasemy, E**., Zeraati, A. S., ... & Mirhashemi, A. **(2021)**. In situ simultaneous chemical activation and exfoliation of carbon quantum dots for atmospheric adsorption of H2S and CO2 at room temperature. ***Applied Surface Science***, *559*, 149892.

9. **Ghasemy, E**., Emrooz, H., Rashidi, A., & Hamzehlouyan, T. **(2020)**. Highly uniform molybdenum oxide loaded N-CNT as a remarkably active and selective nanocatalyst for H_2S selective oxidation. ***Science of The Total Environment***, 711, 134819.

10. Khoshoei, A†., **Ghasemy, E**†., Poustchi, F., Shahbazi, M. A., & Maleki, R. **(2020)**. Engineering the pH-Sensitivity of the Graphene and Carbon Nanotube Based Nanomedicines in Smart Cancer Therapy by Grafting Trimetyl Chitosan. ***Pharmaceutical Research***, *37*(8), 1-13. (†: the same contribution)

11. Daraee, M., **Ghasemy, E**., & Rashidi, A. **(2020)**. Effective adsorption of hydrogen sulfide by intercalation of TiO2 and N-doped TiO2 in graphene oxide. ***Journal of Environmental Chemical Engineering***, *8*(4), 103836.

12. Daraee, M., **Ghasemy, E.**, & Rashidi, A. **(2020)**. Synthesis of novel and engineered UiO-66/graphene oxide nanocomposite with enhanced H2S adsorption capacity. ***Journal of Environmental Chemical Engineering***, 8(5), 104351.

13. Yousefian, Z., **Ghasemy, E**., Askarieh, M., & Rashidi, A. **(2019)**. Theoretical studies on B, N, P, S, and Si doped fullerenes toward H2S sensing and adsorption. ***Physica E: Low-dimensional Systems and Nanostructures***, *114*, 113626.

14. Alivand, M., Shafiei-Alavijeh, M., Tehrani, N., **Ghasemy, E**., Rashidi, A., & Fakhraie, S. **(2019)**. Facile and high-yield synthesis of improved MIL-101 (Cr) metal-organic framework with exceptional CO_2 and H_2S uptake; the impact of excess ligand-cluster. ***Microporous and Mesoporous Materials***, *279*, 153-164.

15. Alivand, M., Najmi, M., Tehrani, H., Kamali, A., Tavakoli, O., Rashidi, A., Esrafili, M., **Ghasemy, E**., Mazaheri, O. **(2019)**. Tuning the surface chemistry and porosity of waste-derived nanoporous materials toward exceptional performance in antibiotic adsorption: Experimental and DFT studies. ***Chemical Engineering Journal***, *374*, 274-291.

16. **Ghasemy, E**., Motejadded, H., Rashidi, A., Hamzehlouyan, T., & Yousefian, Z. **(2018)**. N-doped CNT nanocatalyst prepared from camphor and urea for gas phase desulfurization: experimental and DFT study. Journal of the ***Taiwan Institute of Chemical Engineers***, 85, 121-131.

17. Pourhashem, S., **Ghasemy, E**., Rashidi, A., & Vaezi, M. R. **(2018)**. Corrosion protection properties of novel epoxy nanocomposite coatings containing silane functionalized graphene quantum dots. ***Journal of Alloys and Compounds***, *731*, 1112-1118.

18. Hassani, S. S., Samiee, L., **Ghasemy, E**., Rashidi, A., Ganjali, M. R., & Tasharrofi, S. **(2018)**. Porous nitrogen-doped graphene prepared through pyrolysis of ammonium acetate as an efficient ORR nanocatalyst. ***International Journal of Hydrogen Energy***, *43*(33), 15941-15951.

19. Madannejad, S., Rashidi, A., Sadeghhassani, S., Shemirani, F., & **Ghasemy, E**. **(2018)**. Removal of 4-chlorophenol from water using different carbon nanostructures: a comparison study. ***Journal of Molecular Liquids***, *249*, 877-885.

20. Pourhashem, S., Rashidi, A., Vaezi, M. R., Yousefian, Z., & **Ghasemy, E**. **(2018)**. The effect of polycrystalline graphene on corrosion protection performance of solvent based epoxy coatings: Experimental and DFT studies. ***Journal of Alloys and Compounds***, *764*, 530-539.

21. Keshtkar, S., Rashidi, A., Kooti, M., Askarieh, M., Pourhashem, S., **Ghasemy, E**., & Izadi, N. **(2018)**. A novel highly sensitive and selective H2S gas sensor at low temperatures based on SnO_2 quantum dots-C60 nanohybrid: experimental and theory study. ***Talanta***, *188*, 531-539.

Books:

- Translation of the book "Hummel, Rolf E. Electronic Properties of Materials. Springer, New York, NY, 2011. 3-5, to Persian, published in Apr. 2016.

Work and Research Experiences

1- INRS University

PhD Student (Jan. 2021-) Supervisors: Prof. Kulbir Kaur Ghuman and Prof. Ana C. Tavares

- Performing DFT calculations to investigate the electrochemical properties of emerging 2-dimensional nanostructures.

2- Khwarizmi Technology Development Company (Iran)

R&D Supervisor/Project Manager (Mar. 2019- Dec. 2021)

- Developing the nanocatalysts for reforming the natural gas and producing syngas based on loading the active nickel phase over the metal oxides and studying the feasibility of commercializing the newly-developed catalysts.
- Project manager of production of different coke morphologies, designing and deploying mini-delayed-coking unit.
- Supervising the thorough characterization of the catalysts which are being developed by other R&D members.
- Developing new desulfurization techniques to reduce the total sulfur of heavy aromatic oils via synthesizing ODS catalysts.
- Supervising and managing the knowledge management section of the company and publishing the patents and scientific reports.
- Designing and fabricating the laboratory scale setup and an industrial scale pilot for mass production of carbonaceous materials.
- Managing the computational section of the company to study the adsorbents and catalysts by DFT calculations prior to the experiments.

3- Research Institute of Petroleum Industry (RIPI)

Research assistant (Jan. 2015- Oct. 2017)**;** Supervisor: Prof. Rashidi

- Synthesis of graphene, Carbon nanotubes, and their N, S, P, and B doped species from low-cost precursors through CVD method for different applications;
- Synthesizing metal-free nano-catalysts for ORR reaction (tuning the nanoporous graphene through N, S, and P doping and using different synthesis methods, for better ORR performance)
- Preparation of corrosion protection nanocomposite coatings by employing various types of graphene and different functionalizing methods (graphene/polymer nanocomposites)
- Synthesizing different carbonaceous adsorbents (i.e. porous carbon, carbon nanofiber, CNTs, graphene, and carbon quantum dots) for removing 4-chlorophenol from water
- Computational materials science to predict catalytic, adsorptive, sensing, and corrosion inhibiting properties of novel materials through Density Functional Theory (DFT) (i.e. Gaussian and Materials Studio software)
- Developing novel and efficient sensors to detect H_2S via DFT calculations and experiments
- Synthesizing MIL-101 (Cr) for adsorption of CO_2 and H_2S (Metal Organic Frameworks (MOFs))

3- Iran University of Science and Technology and Research Institute of Petroleum Industry (RIPI)

M.Sc. student (Jan. 2014- Dec. 2016)

Supervisors: Dr. Banna Motejadded, Prof. Rashidi, and Dr. Hamzehlouyan

- Synthesis of Carbon Nanotubes (CNTs) by using different growth catalysts and precursors.
- Synthesis of Nitrogen doped CNTs through CVD method by using low-cost and abundant solid precursors.
- Synthesis of Molybdenum oxides loaded N-CNTs through incipient wetness impregnation.
- Investigation on application of the prepared metal-free and metal oxide nanocatalysts in selective oxidation of H_2S by performing reactor tests.
- Characterizing the prepared Nanocatalysts in collaboration with Instituto de Nanociencia de Aragón, Zaragoza University, Spain.
- Performing DFT calculations to determine the active phases in H_2S removal.

Computer and Language Skills

- **Computational software:**

Quantum Espresso, Quantum ATK, Gaussian, Gaussview, Materials Studio, and Spartan;

- **Other Software:**

Origin, CasaXPS, and Spectral Data Processor (SDP), and Sigmaplot;

- **Knowledge management tools:**

Mendeley and EndNote software, Scopus, WebofScience, and google scholar websites.

TOEFL IBT

MyBestScore; Total score: 96; Reading: 27; Listening: 25; Speaking: 23; and Writing: 21.

Research Interests

- General Materials Science
- Nanotechnology and Nanomaterials
- Carbon Nanostructures (CNTs and Graphene)
- Computational Materials Science
- Nano-Catalysis and Computational Catalysis
- Environmental Nanotechnology
- Energy Materials

Scientific Services

Institute of Materials and Energy (MERC), Karaj, Iran

- Grammatical editor of ISC Journal of "Advanced Ceramics Progress (ACERP)" (Link) Jul. 2016- Jul. 2017
- Grammatical editor of ISC "Journal of Renewable Energy and Environments (JREE)" (Link) Jul. 2016-Jul-2017

References

1. **Prof. Kulbir Kaur Ghuman**
   Énergie Matériaux Télécommunications Research Centre, at Institut National de la Recherché Scientifique (INRS)
   kulbir.ghuman@inrs.ca

2. **Prof. Ana C. Tavares**
   Énergie Matériaux Télécommunications Research Centre, at Institut National de la Recherché Scientifique (INRS)
   ana.tavares@inrs.ca

3. **Prof. Alimorad Rashidi**
   Research Institute of Petroleum Industry (RIPI), Tehran, Iran
   Rashidiam@ripi.ir