Dr. Pezhman Zarabadi-Poor, Ph.D.

Computational Materials Scientist

Department of Chemistry, University of Bath, Bath, United Kingdom

Summary

I am eager in benefiting from the synergy between my computational skills and experimental background to tackle challenging energy and environmental obstacles at the intersection of material and computational science. I have developed the experimental skills throughout my MSc and PhD studies while I have learned computational techniques after my PhD on my own interest and effort. Although I am able to conduct independent research projects, I thrive working as a team member and have proactively collaborated with researchers at different institutions around the world to complete various projects.

Education

University of Tehran   *Tehran, Iran*

Ph.D. in Inorganic Chemistry   *Oct. 2008 - May 2013*

- Specialized on synthesis of carbon nanotubes (solvothermal) surface modification of mesoporous silicas

University of Tehran   *Tehran, Iran*

M.Sc. in Inorganic Chemistry   *Oct. 2006 - Sep. 2008*

- Specialized on Synthesis and characterization of carbon nanotubes (CCVD method) and mesoporous silicas

Bu-Ali Sina University   *Hamedan, Iran*

B.Sc. in Applied Chemistry   *Oct. 2002 - Sep. 2006*

- Got the chance to work in oil refinery as internship

National Organization for Development of Exceptional Talents   *Qazvin, Iran*

Diploma   *Oct. 1997 - Sep. 2002*

Work Experience

University of Bath   *Bath, United Kingdom*

Research Associate   *June 2020 - Current*

- Research associate in CATMAT project

Central European Institute of Technology - Masaryk University   *Brno, Czechia*

MarieSkłodowska-Curie Postdoctoral Fellow   *Apr. 2017 - Apr. 2020*

- Principal Investigator of COMPSTORE project

National Autonomous University of Mexico   *Mexico City, Mexico*

DGAPA Postodoctoral Fellow   *Mar. 2016 - Apr. 2017*

- Implementing the biogas upgrading project

Helmholtz - Center of Environmental Research (UFZ)   *Leipzig, Germany*

Research Stay   *Jul. 2010 - Sep. 2010*

- Wet peroxide oxidation of organic pollutants

Behineh Kala Gostar   *Tehran, Iran*

Techinal staff   *2008 - 2012*

- Installation and service of BEL gas adsorption instruments

Pars Pamchal Paint factory   *Qazvin, Iran*

R & D Researcher   *Jun. 2011 - Dec. 2013*

- Developing different types of water resistant paints

Arak Oil refinery   *Arak, Iran*

Undergraduate Internship   *Jun. 2011 - Dec. 2013*

- Working in different parts of QC lab

Publications:

Pre-prints and in-process:

2021   P. Zarabadi-Poor, B. J. Morgan, and M. S. Islam, *Accelerated Discovery of Next-Generation Cathode Materials for Li-ion Batteries*, **CATMAT**, In-Preparation

2021   P. Zarabadi-Poor, X. Wang, J. Bocarsly, J. Lim, L. Daniels, R. Chen, B. J. Morgan, C. Grey, M. Rosseinsky, and M. S. Islam, *Designing, Synthesis, and Characterization of Novel Sulphide Cathode Materials*, **CATMAT**, In-Preparation

2021   P. Zarabadi-Poor, N. Bryan, B. J. Morgan, and M. S. Islam, *Designing Li-rich Novel Sulphide Cathodes using Li intercalation*, **CATMAT**, In-Preparation

2021   H. Richards, P. Zarabadi-Poor, B. J. Morgan, and M. S. Islam, *In-Silico Exploration of Potential Next-Generation Cathodes for Li-ion Batteries*, **CATMAT**, In-Preparation

2021   S. P. Huber, E. Bosoni, M. Bercx, J. Bröder, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, A. Garcia, L. Genovese, D. Gresch, C. Johnston, G. Petretto, S. Poncé, G.-M. Rignanese, C. J. Sewell, B. Smit, V. Tseplyaev, M. Uhrin, D. Wortmann, A. V. Yakutovich, A. Zadoks, P. Zarabadi-Poor, B. Zhu, N. Marzari, and G. Pizzi, *Common workflows for computing material properties using different quantum engines*, 2021 - arXiv - Submitted

2021   P. Zarabadi-Poor, *Screening and Detailed Atomistic Investigation of CoRE MOFs for Xenon Recovery from Exhaled Anesthetic Gas*, In-Preparation

2021   P. Zarabadi-Poor, *Helium Capture inside NMR Machine: An Alternative Solution for Helium Recovery*, In-Preparation

Peer-reviewed:

2020   O. Jurček, R. Puttreddy, F. Topić, P. Jurček, P. Zarabadi-Poor, H. V. Schröder, R. Marek, and K. Rissanen, *Heads or tails? sandwich-type metallocomplexes of hexakis (2, 3-di-o-methyl)-α-cyclodextrin*, Crystal Growth & Design, (2020)

2019   P. Zarabadi-Poor and R. Marek, *Metal–Organic Frameworks for Helium Recovery from Natural Gas via N_2/He Separation: A Computational Screening*, The Journal of Physical Chemistry C, 123 (2019), pp. 3469–3475

2019   P. Zarabadi-Poor and R. Marek, *Comment on "Database for CO_2 Separation Performances of MOFs Based on Computational Materials Screening"*, ACS applied materials & interfaces, 11 (2019), pp. 16261–16265

2018   S. Panter and P. Zarabadi-Poor, *Computational Exploration of IRMOFs for Xenon Separation from Air*, ACS Omega, 3 (2018), pp. 18535–18541

2018   P. Zarabadi-Poor and R. Marek, *In Silico Study of (Mn, Fe, Co, Ni, Zn)-BTC Metal–Organic Frameworks for Recovering Xenon from Exhaled Anesthetic Gas*, ACS Sustainable Chemistry & Engineering, 6 (2018), pp. 15001–15006

2018   P. Zarabadi-Poor and T. Rocha-Rinza, *A Detailed Atomistic Molecular Simulation Study on Adsorption-Based Separation of CO_2 Using a Porous Coordination Polymer*, RSC advances, 8 (2018), pp. 14144–14151

2017   L. Hajiaghababaei, S. Abozari, A. Badiei, P. Zarabadi-Poor, S. Dehghan Abkenar, M. R. Ganjali, and G. Mohammadi Ziarani, *Amino Ethyl-Functionalized SBA-15: A Promising Adsorbent for Anionic and Cationic Dyes Removal*, Iranian Journal of Chemistry and Chemical Engineering (IJCCE), 36 (2017), pp. 97–108

2015   M. Karimi, A. Badiei, and P. Zarabadi-Poor, *The Impact of Cadmium Loading In Fe/Alumina Catalysts and Synthesis Temperature on Carbon Nanotubes Growth by Chemical Vapor Deposition Method*, Journal of Sciences, Islamic Republic of Iran, 26 (2015), pp. 17–24

2014   A. Shahbazi, R. Gonzalez-Olmos, F.-D. Kopinke, P. Zarabadi-Poor, and A. Georgi, *Natural and Synthetic Zeolites in Adsorption/Oxidation Processes to Remove Surfactant Molecules from Water*, Separation and Purification Technology, 127 (2014), pp. 1–9

2014   P. Zarabadi-Poor and J. Barroso-Flores, *Theoretical Assessment of the Selective Fluorescence Quenching of 1-amino-8-naphthol-3, 6-disulfonic acid (H-acid) Complexes with Zn^{2+}, Cd^{2+}, and Hg^{2+}: a DFT and TD-DFT Study*, The Journal of Physical Chemistry A, 118 (2014), pp. 12178–12183

2013   P. Zarabadi-Poor, A. Badiei, A. A. Yousefi, and J. Barroso-Flores, *Selective Optical Sensing of Hg(II) in Aqueous Media by H-Acid/SBA-15: A Combined Experimental and Theoretical Study*, The Journal of Physical Chemistry C, 117 (2013), pp. 9281–9289

2013   P. Zarabadi-Poor, A. Badiei, and A. A. Yousefi, *Synthesis of Novel Carbon Nanostructures through Solvothermal Route*, Scientia Iranica, 20 (2013), pp. 2382–2385

2012   L. Hajiaghababaei, A. Badiei, M. Shojaan, M. Ganjali, G. Ziarani, and P. Zarabadi-Poor, *A Novel Method for the Simple and Simultaneous Preconcentration of Pb^{2+}, Cu^{2+} and Zn^{2+} Ions with Aid of Diethylenetriamine Functionalized SBA-15 Nanoporous Silica Compound*, International journal of environmental analytical chemistry, 92 (2012), pp. 1352–1364

2012   L. Hajiaghababaei, S. Kazemi, A. Badiei, P. Zarabadi-Poor, M. R. Ganjali, and G. M. Ziarani, *Using the Hydroxymethyl-Modified Nanoporous Silica as a PVC Membrane Electrode Modifier to Determination of Lead Ions*, Analytical and Bioanalytical Electrochemistry, 4 (2012), pp. 246–261

2011   G. Mohammadi Ziarani, A. Badiei, M. Azizi, and P. Zarabadi-Poor, *Synthesis of 3,4-dihydropyrano [c] Chromene Derivatives using Sulfonic Acid Functionalized Silica (SiO_2PrSO_3H)*, Iranian Journal of Chemistry and Chemical Engineering (IJCCE), 30 (2011), pp. 59–65

2011   P. Zarabadi-Poor, A. Badiei, B. D. Fahlman, P. Arab, and G. Mohammadi Ziarani, *One-pot Synthesis of Ethanolamine-modified Mesoporous Silica*, Industrial & Engineering Chemistry Research, 50 (2011), pp. 10036–10040

2011   P. Zarabadi-Poor and A. Badiei, *Synthesis of Carbon Nanotubes using Metal-modified Nanoporous Silicas*, Carbon Nanotubes-Growth and Applications, (2011), pp. 59–74

2010   P. Zarabadi-Poor, A. Badiei, A. A. Yousefi, B. D. Fahlman, and A. Abbasi, *Catalytic Chemical Vapour Deposition of Carbon Nanotubes using Fe-doped Alumina Catalysts*, Catalysis Today, 150 (2010), pp. 100–106

2009   P. Hashemi, M. Shamizadeh, A. Badiei, P. Zarabadi-Poor, A. R. Ghiasvand, and A. Yarahmadi, *Amino Ethyl-functionalized Nanoporous Silica as a Novel Fiber Coating for Solid-phase Microextraction*, Analytica chimica acta, 646 (2009), pp. 1–5

Workshops and Trainings

AiiDA Hackathon   *Bologna, Italy*
Developing Code Plugins and Robust Scientific Workflows   *Feb. 2020*

MSSC2019 - CRYSTAL17 Workshop   *London, UK*
Ab initio Modelling in Solid State Chemistry   *Sep. 2019*

AiiDA Workshop   *Lausanne, Switzerland*
Writing Reproducible Workflows with AiiDA   *May 2019*

RASPA Workshop   *Delft, Netherlands*
Molecular simulations for adsorption/diffusion in nanoporous materials and modeling of ionic liquids   *Jun. 2018*

At the heart of MOF chemistry: Topology   *Munich, Germany*
Workshop on using TOPOSPRO Software   *Nov. 2018*

Leadership Course by hfp   *Brno, Czechia*
Professional Development for Young Scientists Course   *Nov. 2018*

Funding

Marie Skłodowska-Curie/SoMoPro COFUND   *CEITEC-MU, Brno, Czechia*
207,000.00 Euro - 36 months   *Apr. 2017 - Apr. 2020*
- Advanced Carbon@MOF Composites for Gas Storage and Separation

DGAPA Postdoctoral Fund   *UNAM, Mexico*
360,000.00 MXN (20,000.00 USD)- 12 month   *Mar. 2016 - Apr. 2017*
- Computer Simulation of MOFs for Biogas Upgrading

Iranian Nanotechnology Innovation Council   *Tehran, Iran*
Scholarship   *2011*
- Financial support of PhD thesis

Iranian Nanotechnology Innovation Council   *Tehran, Iran*
Scholarship   *2008*
- Financial support of MSc thesis

Collaborations

CURRENT:

Prof. Berend Smit and Dr. Daniele Ongari   *EPFL, Switzerland*

Topic: Noble Gas Separation   *May 2019 - now*

- Accelerating the High-throughput Screening by Developing Novel Pre-selection Descriptors

Prof. Christopher Wilmer   *University of Pittsburgh, USA*

Topic: Carbon Capture   *2016 - now*

- Investigation of CO_2 Adsorption on Thermal Conductivity of MOF-177 series

PAST:

Prof. Bradley Fahlman   *Central Michigan University, USA*

Topic: Nanomaterials Synthesis   *2008 - 2010*

- Synthesis and Characterization of CNTs and Funcionalized Mesoporous Silicas

Dr. Joaquin Barroso-Flores   *UNAM, Mexico*

Topic: Optical Sensors   *2008 - 2010*

- Computational Exploration of Fluorescence Quenching in Mercury Sensors

Technical Skills & Software

Programming	Advanced: Python
	Learning: C/C++, LaTex
Codes and Software	RASPA, Zeo++, Gaussian, CP2K, AIMALL, LAMMPS, Chargemol, VASP, AiiDA, CRYSTAL17, pyIAST, ORCA, LOBSTER
aiida-bjm	Author: Collection of AiiDA Workchains for Cathode Material Discovery - **CATMAT**
aiida-sqs	Author: AiiDA Plugin for Generation of SQS - **CATMAT**
aiida-nmr	Author: AiiDA Workflows for Simulation of NMR Chemical Shifts in Cathode Materials - **CATMAT**
aiida-porousmaterials	Author: AiiDA Plugin for PorousMaterials package
aiida-MatDis	Author: Collection of AiiDA Workchains for Materials Discovery
aiida-orca	Author: AiiDA Plugin for ORCA package
aiida-raspa	Contributor: AiiDA plugin for RASPA package
aiida-zeopp	Contributor: AiiDA plugin for Zeo++ Package
aiida-cp2k	Contributor: AiiDA plugin for CP2K package
Zeo++	Contributor: Improved a feature in the code

Supervision and Scientific Consultancy

Hollie Richards   *University of Bath, Bath, UK*

PhD Student   *Apr. 2021 - Current*

- In-Silico Design of Next-generation Cathode Materials

Noah Bryan   *University of Bath, Bath, UK*

Last Year Bachelor Student   *Nov. 2020 - Apr. 2021*

- Computational Investigation of Candidate Prototypes for Designing Next-Generation Cathode Materials

Sabrina Panter   *CEITEC-MU, Brno, Czechia*

visiting DAAS-RISE BSc student   *Aug. 2018 - Sep. 2018*

- Xenon Recovery from Air using MOFs

Mahya Asgharian Marzabad   *CEITEC-MU, Brno, Czechia*

Materials Chemistry PhD student   *Jan. 2019 - Current*

- Optimization of Synthesis Variables of Selected MOFs for Noble Gas Separation