

Sahar Bayat

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EDUCATION AND TRAINING

[22/08/2022 – Current]

PhD Materials Chemistry, Supervisor: Prof. Chad Risko

University of Kentucky

City: Lexington

Country: United States

Final grade: 3.76/4

[20/09/2018 – 12/11/2020]

MS Catalysis Chemistry, Supervisor: Prof. S.Shahab Naghavi

Shahid Beheshti University

City: Tehran

Country: Iran

Final grade: Excellent

Thesis: Silver chalcogenides 2DCs application in photocatalytic water splitting based on DFT

[19/09/2010 – 28/01/2015]

BS Applied Chemistry

Shahid Beheshti University

City: Tehran

Country: Iran

PROJECTS

[01/05/2023 – Current]

Evaluation of structural properties in amorphous Mo₃S₁₃ chalcogel-based electrodes for Li/Na ion batteries through ab initio molecular dynamics in VASP

Applying AIMD-MQ simulations, this project aims to evaluate bond lengths in amorphous Mo₃S₁₃. By analyzing the pair correlation function (PCF) $g(r)$, insights into local atomic arrangements and bonding environments are sought, aiding in understanding Mo-Mo, Mo-S, and S-S distances.

University of Kentucky, Dr. Chad Risko

[01/02/2024 – Current]

Simulating x-ray absorption spectroscopy (XAS) K- & L-edges of (NH₄)₂Mo₃S₁₃ in VASP

This project aims to calculate X-ray absorption spectroscopy (XAS) K- & L-edges in (NH₄)₂Mo₃S₁₃ using the supercell core-hole (SCH) method. By examining XAS spectra, insights into local structure and bonding properties of molybdenum and sulfur coordination are anticipated.

University of Kentucky, Dr. Chad Risko

[19/08/2018 – 11/11/2020]

DFT study of 2D silver chalcogenide and their application in photocatalytic water splitting

Shahid Beheshti University, Dr. Shahab Naghavi

[20/07/2018 – 20/07/2022]

Synthesis and characterization of high performance polycarboxylate superplasticizer (PCE) for application in concrete admixtures

Abadgaran Construction Chemical Manufacturer, R&D Dept.

PATENT

[20/01/2022] **Modified carboxylate/vinyl ester copolymers for concrete admixtures**

Publication :**WO2022013600A1**, A-2022-01-20, Application : **IB2020056651WA**-2020-07-15

T. Salemnoush, **S.Bayat**, A. M. Hosseini

PUBLICATIONS

[2024]

Mo3S13 Chalcogel: A High-Capacity Electrode for Conversion-Based Li-ion Batteries

Islam, T.; Roy, S. C.; **Bayat, S.**; Weret, M. A.; Hoffman, J. M.; Rao, K. R.; Sawicki, C.; Nie, J.; Alam, R.; Oketola, O. Mo3S13 Chalcogel: A High-Capacity Electrode for Conversion-Based Li-ion Batteries. *ChemSusChem* **2024**, e202400084.

[2023]

Chalcocarbogels as High-Capacity and Cycle-Stable Electrode Materials for Lithium and Sodium Ion Batteries

Islam, T.; Li, M.; Blanton, A.; Pitton, K. A.; Rao, K. R.; **Bayat, S.**; Wiaderek, K. M.; Weret, M. A.; Roy, S. C.; Feng, R. Chalcocarbogels as High-Capacity and Cycle-Stable Electrode Materials for Lithium and Sodium Ion Batteries. *ACS Energy Letters* **2023**, 9 (1), 1-9.

[2020]

Ethyl ester of vegetable oil derived carboxy-imidazoline drilling corrosion inhibitor

National Intellectual Property Center of the Islamic Republic of Iran

[2021]

Efficient method for synthesizing 4,4'-Methylenedianiline by reduction of aromatic nitro compounds

National Intellectual Property Center of the Islamic Republic of Iran

[2020]

Superplasticizer admixture of amphoteric copolymers of styrene an maleic anhydride with superior water reduction ability

National Intellectual Property Center of the Islamic Republic of Iran

CONFERENCES AND SEMINARS

[28/03/2024]

49th Annual Naff Symposium, Poster presentation: Structural properties in amorphous molybdenum sulfide materials of interest for Li-S batteries

Lexington, Ky

Sahar Bayat, Keerthan R. Rao, Taohedul Islam, Saiful M. Islam, and Chad Risko (*Poster Presentation*)

[04/2024]

Structural Properties and Ion Diffusion Pathways in Molybdenum Sulfide Materials of Interest for Li-S Batteries

Materials Research Society, Spring 2024

Sahar Bayat, Keerthan R. Rao, Taohedul Islam, Saiful M. Islam, and Chad Risko (*Poster Presentation*)

[03/2024]

Chalco-carbogels as high capacity and cycle-stable electrode materials for lithium- and sodium-ion batteries

ACS Spring 2024

T. Islam, M. Li, A. Blanton, K. Pitton, K. Rao, **S. Bayat**, K. Wiaderek, M. Weret, S. Roy, R. Feng, D. Li, R. Alam, J. Nie, O. Oketola, A. Pramanik, B. Guiton, C. Risko, I. Belharouak, R. Amin, S. Islam

[10/2024]

Chalcogenide-Based Gels As High-Capacity Electrodes for Lithium-Ion Batteries

The Electrochemical Society PRiME 2024

S. M. Islam, I. Taohedul, M. Weret, S. Roy, **S. Bayat**, K. Rao, M. Li, C. M. Risko, K. Wiaderek, and R. Amin (*Oral Presentation*)

[09/01/2019]

5th national conference on presentation of " A Review of Redox and Thermal Initiation in Free Radical Polymerization"

Shahid Beheshti University

[09/01/2019]

5th national conference on presentation of " A review of industrial heterogeneous catalysis esterification"

Shahid Beheshti University

[19/02/2018]

5th international conference on presentation of " Evaluation of water based, non-corrosive and eco-friendly form release agent"

Amirkabir University of Technology

HONOURS AND AWARDS

[28/03/2024] **Naff Symposium 2nd Place Poster Presentation** Awarding institution: University of Kentucky

[15/02/2022] **Mark and Ruth Luckens Graduate Fellowship** Awarding institution: University of Kentucky

WORK EXPERIENCE

[12/05/2023 – Current] **University research assistant**

University of Kentucky

City: Lexington

Country: United States

- Reviewing published literature, designing, and conducting simulations
- Analyzing and summarizing results, preparing reports
- Attending regular project progress and discussion meetings

[20/08/2022 – 20/12/2023]

University teaching assistant

University of Kentucky

City: Lexington

Country: United States

- Instruct students organic chemistry laboratory (CHE 233) course
- Adhering to departmental approved course outlines and syllabi, using approved text and other instructional materials
- Meeting with supervisor and other TAs on a regular basis
- Grading class materials
- Meeting and assisting individual students during office hours

[29/06/2017 – 20/07/2022]

Research chemist

Abadgaran Chemical Technology Development Research Group

City: Tehran

Country: Iran

Email address: s.bayat@abadgarangroup.com

Name of unit or department: Research and Development

Business or sector: Manufacturing

1. **Research project on energy engineering in construction by means of synthesizing Superplasticizers/Water reducer additives for concrete**
2. **Research project on synthesis of vegetable oil based curing agents for application in adhesives, coatings, sealants, filler, floor and flooring repair, encapsulation**
3. **Research project on synthesis of heterocyclic imidazoline compounds for application in drilling corrosion inhibitors**
4. **Research project on synthesis of isothiazolinone as an antimicrobials and preservatives**

Including tasks:

- Synthesizing compounds and developing analytical and chemical test methods for characterization.
- Recording and analyzing data based on researches and studies.
- Researching and writing papers, patents, reports and reviews.
- Participating in conferences, presenting and related exhibitions.
- Supervising junior staff, including junior researchers, and laboratory technicians.

[21/09/2015 – 30/06/2017]

Research chemist

Chito Tech Company

City: Tehran

Country: Iran

Name of unit or department: Research and Development

Business or sector: Manufacturing

Conducting research project on wound dressing and hemostatic based on silver nanoparticles

Including tasks:

- Designing new wound dressings based on colloidal silver technology as an effective antiseptic agent.
- Fabricating chitosan and chitin based hybrid materials for treatments of chronic or/and acute burn wounds.
- Collecting and analysis of project required technical specification in accordance with Iranian Ministry of Health as well as CE, ISO13485 standards.
- Designing and conducting tests and experiments for analyzing syntheses products as well as raw materials.
- Designing new formulation for hygiene products by compounding various natural biopolymers.

- Conducting compound analysis by applying spectrophotometry methods and determining the physical and chemical properties.
- Making sure that all GMPs, regulatory mandates and quality requirements are correctly met.

DIGITAL SKILLS

First-Principles Simulation: VASP, Quantum Espresso | Programming languages (Python and R program)

LANGUAGE SKILLS

Mother tongue(s): Persian

Other language(s):

English

LISTENING C1 READING C1 WRITING B2

SPOKEN PRODUCTION C1 SPOKEN INTERACTION C1

French

LISTENING B2 READING B1 WRITING B1

SPOKEN PRODUCTION B1 SPOKEN INTERACTION B2

Spanish

LISTENING B1 READING A2 WRITING A1

SPOKEN PRODUCTION A2 SPOKEN INTERACTION B1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user