Sahar Bayat

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Address: Lexington, United States (Home)

EDUCATION AND TRAINING

22/08/2022 - CURRENT Lexington, United States

PHD CANDIDATE MATERIALS CHEMISTRY, SUPERVISOR: PROF. CHAD RISKO University of Kentucky

20/09/2018 - 12/11/2020 Tehran, Iran

MS CATALYSIS CHEMISTRY, SUPERVISOR: PROF. S.SHAHAB NAGHAVI Shahid Beheshti University

19/09/2010 - 28/01/2015 Tehran, Iran

BS APPLIED CHEMISTRY Shahid Beheshti University

PROJECTS

01/05/2023 - CURRENT

Evaluation of Structural Properties in MoxSy Chalcogel-Based Electrodes for Li/Na Ion Batteries Using Ab Initio Molecular Dynamics (AIMD)

• Developing AIMD approaches to evaluate structural properties such as radial distribution functions, bond lengths, and coordination numbers in MoxSy-based chalcogels. Analyzing these features provides insights into the local atomic arrangements and bonding environments of these materials, which aids in undesrtanding structure-property relationships.

University of Kentucky, Dr. Chad Risko

01/02/2024 - CURRENT

Determing K- and L-edges of Mo and S in Amorphous MoxSy Chalcogel-Based Electrodes by Means of X-ray Absorption Spectroscopy (XAS) Ab Initio Simulations

 Developing computational approaches to explore XAS in amorphous MoxSy derivatives using the supercell corehole (SCH) method. This project provides insights into how local structure and bonding impact electronic characteristics crucial to redox activity.

University of Kentucky, Dr. Chad Risko

19/08/2018 - 11/11/2020

Density Functional Theory (DFT) Investigation of Single Layer Transition Metal Chalcogenides (TMCs) for Their Application in Photocatalytic Water Splitting

 Establishing a computational approach to determine electronic properties such as band gap, density of states, absorption characteristics, thermodynamic stability and other electronic features in 2D silver chalcogenides as novel photocatalysts for photocatalytic water splitting. Analyzing these properties aids in developing innovative catalysts for energy conversion materials.

Shahid Beheshti University, Dr. Shahab Naghavi

20/07/2018 - 20/07/2022

Synthesis and Characterization of High-Performance Polycarboxylate Superplasticizers (PCEs) for use in Concrete Admixtures

• Developing novel synthesis routes for industrial-scale production of plasticizers and superplasticizers for use in construction. These materials help with the workability and signifficantly reduce the water-to-cement ratio, contributing to environmental sustainability.

Abadgaran Construction Chemical Manufacturer, R&D Department

PATENT

20/01/2022

Modified carboxilate/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

202

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

04/2024 Materials Research Society, Spring 2024, Seattle, WA

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

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

28/03/2024 Lexington, KY

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

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

09/01/2019 Shahid Beheshti University

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

09/01/2019 Shahid Beheshti University

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

19/02/2018 Amirkabir University of Technology

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

HONOURS AND AWARDS

26/04/2024

Fast Start Award - University of Kentucky

Naff Symposium 2nd Place Poster Presentation – University of Kentucky

15/02/2022

Mark and Ruth Luckens Graduate Fellowship - University of Kentucky

WORK EXPERIENCE

12/05/2023 - CURRENT Lexington, United States

UNIVERSITY RESEARCH ASSISTANT UNIVERSITY OF KENTUCKY

- Review published literature to design and conduct modeling-based experiments
- Analyze and summarize results to preparing reports, papers, and presentations
- Attend and present at regular project progress meetings

20/08/2022 - 20/12/2023 Lexington, United States

UNIVERSITY TEACHING ASSISTANT UNIVERSITY OF KENTUCKY

- Instruct students organic chemistry laboratory (CHE 233) course
- Adher to departmental approved course outlines and syllabi, using approved text and other instructional materials
- · Meet with supervisor and other TAs on a regular basis
- Grade class materials
- · Meet and assist individual students during office hours

29/06/2017 - 20/07/2022 Tehran, Iran

RESEARCH CHEMIST ABADGARAN CHEMICAL TECHNOLOGY DEVELOPMENT RESEARCH GROUP

- 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:

- Synthesize novel materials and develop analytical and chemical test methods for their characterization.
- Record and analyze research data.
- Write papers, patents, reports, and reviews.
- Participate in conferences, and related exhibitions.
- Supervise junior staff, including junior researchers and laboratory technicians.

Business or Sector Manufacturing | Department Research and Development | Email s.bayat@abadgarangroup.com

21/09/2015 - 30/06/2017 Tehran, Iran

RESEARCH CHEMIST CHITO TECH COMPANY

Conduct research on wound dressing and hemostatic based on silver nanoparticles Including tasks:

- Design new wound dressings based on colloidal silver technology as an effective antiseptic agent.
- Fabricate chitosan and chitin based hybrid materials for treatments of chronic or/and acute burn wounds.
- Collect and analysis of project required technical specification in accordance with Iranian Ministry of Health as well as CE, ISO13485 standards.
- Design and conducting tests and experiments for analyzing syntheses products as well as raw materials.
- Design new formulation for hygiene products by compounding various natural biopolymers.
- Conduct compound analysis by applying spectrophotometry methods and determining the physical and chemical properties.
- Ensure that all GMPs, regulatory mandates and quality requirements are correctly met.

Business or Sector Manufacturing | **Department** Research and Development

DIGITAL SKILLS

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

LANGUAGE SKILLS

Mother tongue(s): **PERSIAN**

Other language(s):

| | UNDERSTANDING | | SPEAKING | | WRITING |
|---------|---------------|---------|--------------------------------------|----|---------|
| | Listening | Reading | Spoken production Spoken interaction | | |
| ENGLISH | C1 | C1 | C1 | C1 | B2 |
| FRENCH | B2 | B1 | B1 | B2 | B1 |
| SPANISH | B1 | A2 | A2 | B1 | A1 |

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