Samira Nikmanesh

Email: nikmanes@mcmaster.ca

50 Glen Road, Hamilton, ON

Phone: 905-601-7960

LinkedIn: linkedin.com/in/samira-nikmanesh

Education

2024
Ph.D. Candidate in Computational Science and Engineering, McMaster University
Supervisor: Dr. Seshasai Srinivasan
Thesis: Investigation of Novel 2D Materials for the Anode of Li-Ion Batteries

2021
Ph.D. in Electronic Engineering, Shiraz University
Supervisor: Dr. Mohammad Hossein Sheikhi
Thesis: Investigation and Simulation of Novel 2D Materials (Phosphorene, Graphyne, g-SiC2) for Methane Nanosensor Applications

2013
M.Sc. in Electronic Engineering, Shiraz University
Supervisor: Dr. Mohammad Hossein Sheikhi
Thesis: Methane Sensor Based on Tin Oxide Nanostructure

2008
B.Sc. in Electronic Engineering, Shiraz University
Supervisor: Dr. Mohammad Hossein Sheikhi
Thesis: DC Motor Drive using AVR Microcontroller

Research Interests

- Lithium-ion and solid-state battery anode materials
- Supercapacitors and energy storage devices
- 2D material design, simulation, and modification
- DFT-based computational materials science
- Solid-state electrolyte interfaces, SEI issues and charge transport

Technical Skills

- DFT Simulation: Quantum ESPRESSO, Atomistix Toolkit
- Programming: Python, C++, Visual C++
- Software: MATLAB, Origin, Microsoft Office
- Characterization Tools: XRD, SEM, XPS, EIS (knowledge and application)
- Hardware/Circuit Design: AVR/8051, Protel DXP, Orcad, PSpice

Research Experience

- Investigation of 2D materials (e.g., SiC, AlN, Phosphorene, Graphyne, g-SiC_2, Stanene) for battery and gas sensing applications
- DFT-Based Study of Phosphorene, Graphyne, AlN, g-SiC and g-SiC_2 as Anode of Li-ion Batteries
- SEI Formation, Solid-State Electrolyte Interfaces, and Charge Transport in Battery Systems
- Fabrication and testing of nanostructured CH_4 sensors
- Interface behavior modeling and analysis for battery electrodes
- Industry project participant in Battery Workforce Challenge McMaster Team (DOE/Stellantis)

Work & Teaching Experience

- Teaching Assistant – Artificial Intelligence, McMaster University (2024–Present)
- Lecturer – Optoelectronics and Semiconductor Devices, Pasargad University (2018–2023)
- Research Member – Cleanroom, NanoTech, and Semiconductor Labs, Shiraz University (2010–2023)

Publications

1. Nikmanesh, S., Srinivasan, S., Safaiee, R., 2025. Ti-decorated SiC2 as a high-performance anode material for Li-ion batteries: A DFT-D2 approach. Mater. Today Phys. 54, 101734. https://doi.org/10.1016/j.mtphys.2025.101734. (Impact Factor: 9.8, Top 10% journal)

2. Nikmanesh, S., Safaiee, R., Sheikhi, M.H., 2022. Enhanced methane-sensing performances of Pd (monomer or dimer) decorated or doped γ-Graphyne: A DFT insight. Surf. Interfaces 29, 101658. https://doi.org/10.1016/j.surfin.2021.101658. (Impact Factor: 6.3)

3. Nikmanesh, S., Safaiee, R., Sheikhi, M.H., 2021. A novel high-performance methane sensor based on Ti-Decorated 2D γ-graphyne: A dispersion-corrected DFT insight. Mater. Chem. Phys. 257, 123808. https://doi.org/10.1016/j.matchemphys.2020.123808. (Impact Factor: 4.7)

4. Nikmanesh, S., Doroodmand, M., Sheikhi, M., 2015. Short Communication Specific Fast Response CH 4 Gas Sensor Based on Metal Oxide, Tungsten Carbide /SnO 2 Core-Shell Modified Interdigitated Electrode.

5. Nikmanesh, S., Doroodmand, M.M., Sheikhi, M.H., Zarifkar, A., Zahabi, A., 2013. Specific CH4 gas sensor based on tungsten carbide/SnO2 core-shell modified interdigitated electrode, in: 2013 21st Iranian Conference on Electrical Engineering (ICEE). Presented at the 2013 21st Iranian Conference on Electrical Engineering (ICEE), pp. 1–7.

References

- Dr. Seshasai Srinivasan, Ph.D., P.Eng.
  Associate Professor, W Booth School of Engineering Practice & Technology
  McMaster University, Hamilton, ON
  Email: ssriniv@mcmaster.ca

I am currently working under Dr. Srinivasan's supervision during my Ph.D. at McMaster, contributing to computational studies of 2D anode materials for lithium-based batteries.

- Dr. Mohammad Hossein Sheikhi
  Professor, Department of Electronics and Telecommunication Engineering
  Shiraz University, Iran
  Email: mshiekhi@shirazu.ac.ir

I conducted my Ph.D. and Master research under the supervision of Prof. Sheikhi, focusing on computational modeling and fabrication of 2D semiconductor materials for advanced gas nanosensing applications.

- Dr. Rosa Safaiee
  Assistant Professor in Physics,
  Shiraz University, Iran
  Email: safaiee@shirazu.ac.ir

Ph.D. advisor; collaborated on computational and experimental research involving 2D semiconductors for gas nanosensor design and Li-ion Battery.