

# Curriculum Vitae

## Personal Information

FIRST NAME: Iman  
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## Current position

- 09/01/2023—now PhD student, Luxembourg Institute of Science and Technology (LIST), Luxembourg.

## Education

- 2015-2018 Master of Science, Shahid Beheshti University (SBU), Department of Energy Engineering, Iran
- 2011-2015 Bachelor of Science, Hormozgan University, Department of Mechanical Engineering, Iran

## Research and Work Experience

- 2018-2022 Senior Programmer, Arta Sanat Co Company, Iran

## Research Activity and Interests

- Computational materials science
- Computational Chemistry
- Data-driven methods in materials science,
- Domain-specific large language models

## Relevant Publications

- Peivaste. et al. Rapid and accurate predictions of perfect and defective material properties in atomistic simulation using the power of 3D CNN-based trained artificial neural networks. *Sci Rep* 14, 36 (2024)
- Peivaste, I., Jossou, E. & Tihamiyu, A.A. Data-driven analysis and prediction of stable phases for high-entropy alloy design. *Sci Rep* 13, 22556 (2023)
- Peivaste, I., et al., Machine-learning-based surrogate modeling of microstructure evolution using phase-field. *Computational Materials Science*, 2022. 214,111750
- Peivaste, I., et al., Comparative study on mechanical properties of three different SiC polytypes(3C, 4H and 6H) under high pressure: First-principle calculations. *Vacuum*, 2018. 154: p. 37-43
- Peivaste, I. and G. Alahyarizadeh, Comparative Study on Absorbed Dose Distribution of Potato and Onion in X-ray and Electron Beam System by MCNPX2. *6 Code. MAPAN*, 2019.34: p. 19-29
- Peivaste, I., et al., Mechanical and thermodynamic properties of 3C structure of silicon carbide using molecular dynamics and density functional theory methods. *Journal of Research on Many-body Systems*, 2019.8: p. 22-38
- A Rezaie, I Peivaste., The Burn-Up raising Feasibility by studying the effects of Th and U contents on the thermophysical and mechanical properties of Th<sub>1-x</sub>U<sub>x</sub>O<sub>2</sub> solid solutions using molecular dynamics. *Progress in Nuclear Energy*, 2021. 134: p 36-44

## Relevant grants and awards

- Academic Full Scholarship, Shahid Beheshti University
- Academic Full Scholarship, Hormozgan University

## Other relevant information