

Saeedeh Kamalinahad

1985-06-23 Iran/Arak

Email: saedehkamalinahad@gmail.com

Current Location: Arak

Phone Number 989186207331

Education

Collaboration:

Kent University

Start-End: 08/2022-08-2023

Post-Doc in Physical Chemistry

Payame Noor University

Start-End: 2022-2023

PhD in Physical Chemistry

Arak University

Start-End: 01/2014 - 09/2018

Sabbatical

University de Barcelona

Start-End date: 09/2017 - 03/2018

MSc in Physical Chemistry

Alzahra University

Start-End date: 09/2010 - 09/2012

BSc in Chemistry

Payam Noor University of Arak

Start-End date: 09/2004 - 01/2008

My thesis

- ✓ Thesis title in **MSc** degree: Theoretical study of interaction between topiramate drug and its derivatives with active site of HCA enzyme by quantum mechanical methods

Thesis director: Dr. Mina Ghiasi

Thesis Reader: Dr. Mansour Zahedi

Defense date: 10/09/2012

Score: 20

GPA: 18.03

- ✓ Thesis title in **PhD** degree: Computational study of nanostructures with optical and gas sensing application

Thesis director: Prof. Mohammad Solimannejad

Thesis Reader: Dr. Ehsan Shakerzadeh

Defense date: 15/09/2018

Score: 20

GPA: 18.69

Teaching

Teacher

1. Arak University, Iran/Arak

Start-End date: 02/2016 - 01/2019

Type of teaching: Official teaching

Name of the course: General Chemistry, Physical Chemistry Laboratory I & II, Solving practice in Quantum chemistry

Type of programme: Bachelor's degree

2. Payam Noor University of Arak, Iran/Arak

Start-End date: 09/2016 - 01/2017

Type of teaching: Official teaching

Name of the course: General Chemistry, General Chemistry Laboratory

Type of programme: Bachelor's degree

Teaching in workshop

1. Name of workshop: Introduction to Gaussian

Organising entity: Arak University

Duration in hours: 8 hours

Start-End date: 04/03/2015 - 04/03/2015

2. Name of workshop: Introduction to Gaussian

Organising entity: Student Chemical Society of Arak University

Duration in hours: 4 hours

Date: 03/2017

Experience Advisor Doctoral thesis

Project title: Theoretical study of adsorption of organic sulfur gases for carbon nitride and silicon nitride nanosheets

Type of project: Doctoral thesis

Entity: Payame Noor University, Zanzan Branch

Student: Mahdi Hoseinali

Date of reading: 06/1401

Scientific production

1. Mina Ghiasi, **Saeedeh Kamalinahad**, Masoud Arabieh, Mansour Zahedi. Carbonic anhydrase inhibitors: A quantum mechanical study of interaction between some antiepileptic drugs with active center of carbonic anhydrase enzyme. Computational and Theoretical Chemistry 992 (2012) 59-69.
Type of production: Scientific paper
Format: Journal
Position of signature: 2
2. Mina Ghiasi, **Saeedeh Kamalinahad**, Mansour Zahedi. Complexation of nanoscale enzyme inhibitor with carbonic anhydrase active center: A quantum mechanical approach. Journal of Structural Chemistry 55 (2014) 1574-1586.
Type of production: Scientific paper
Format: Journal
Position of signature: 2
3. Mina Ghiasi, **Saeedeh Kamalinahad**. Conformational analysis of Topiramate and related anion in the solution and interaction between the most stable conformer of Topiramate with active center of carbonic anhydrase enzyme. Journal of Carbohydrate Chemistry 34 (2015) 80-102.
Type of production: Scientific paper
Format: Journal
Position of signature: 2
4. **Saeedeh Kamalinahad**, Mohammad Solimannejad, Ehsan Shakerzadeh. Sensing of ozone (O_3) molecule via pristine single-walled aluminum nitride nanotube: A DFT study. Superlattices and Microstructures 89 (2016) 390-397.
Type of production: Scientific paper
Format: Journal
Position of signature: 1
5. **Saeedeh Kamalinahad**, Mohammad Solimannejad, Ehsan Shakerzadeh. Nonlinear Optical (NLO) response of pristine and functionalized

Dodecahydrotribenzo[18]annulene ([18]DBA): A theoretical study. Bulletin of the chemical society of Japan 89 (2016) 692-699.

Type of production: Scientific paper

Format: Journal

Position of signature: 1

6. Mohammad Solimannejad, **Saeedeh Kamalinahad**, Ehsan Shakerzadeh. Sensing performance of Sc-doped B₁₂N₁₂ nanocage for detecting toxic Cyanogen gas: A computational study. Physical Chemistry Research 4 (2016) 315-332.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

7. Mohammad Solimannejad, **Saeedeh Kamalinahad**, Ehsan Shakerzadeh. Selective detection of toxic cyanogen gas in the presence of O₂ and H₂O molecules using a AlN nanocluster. Physics Letters A 380 (2016) 2854-2860.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

8. Mohammad Solimannejad, **Saeedeh Kamalinahad**, Ehsan Shakerzadeh. Lin@B₃₆ (n = 1, 2) nanosheet with remarkable Electro-Optical properties: A DFT study. Journal of electronic materials 46 (2017) 4420-4425.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

9. Mohammad Solimannejad, **Saeedeh Kamalinahad**, Ehsan Shakerzadeh. Silicon carbide nanotubes (SiCNTs) serving for catalytic decomposition of toxic diazomethane (DAZM) gas: a DFT study. Molecular Physics 116 (2018) 414-422.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

10. Mohammad Solimannejad, Hamidreza Jouypazadeh, **Saeedeh Kamalinahad**, Motahareh Noormohammadbeigi. Adsorption of F⁻, Cl⁻, Li⁺ and Na⁺ on the exterior surface of Mg₁₂O₁₂ nanocage in the gas Phase and water media: A DFT study. Physical Chemistry Research 4 (2016) 591-605.

Type of production: Scientific paper

Format: Journal

Position of signature: 3

11. Mohammad Solimannejad, **Saeedeh Kamalinahad**, Motahareh Noormohammadbeigi, Hamidreza Jouypazadeh. Chemisorption of Pyrimidine

nucleotide onto exterior surface of pristine B₁₂N₁₂ nanocluster: A theoretical study. Physical Chemistry Research 6 (2018) 1-14.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

12. Mohammad Solimannejad, Forough Rezaie, **Saeedeh Kamalinahad**. Correlating cluster size and NLO response of complexes aggregated with bifurcated metal bonds: a DFT study. Structural Chemistry 29 (2018) 119-127.

Type of production: Scientific paper

Format: Journal

Position of signature: 3

13. Mohammad Solimannejad, Azin Karimi Anjiraki, **Saeedeh Kamalinahad**. Sensing performance of Cu-decorated Si₁₂C₁₂ nanocage towards toxic cyanogen gas: a DFT study. Materials Research Express 4 (2017) 045011.

Type of production: Scientific paper

Format: Journal

Position of signature: 3

14. Mohammad Solimannejad, Rezvan Rahimi, **Saeedeh Kamalinahad**. Nonlinear Optical (NLO) response of Si₁₂C₁₂ nanocage decorated with Alkali metals (M = Li, Na and K): A theoretical study. Journal of Inorganic and Organometallic Polymers and Materials 27 (2017) 1234-1242.

Type of production: Scientific paper

Format: Journal

Position of signature: 3

15. Rezvan Rahimi, **Saeedeh Kamalinahad**, Mohammad Solimannejad. Adsorption of rare gases on the C₂₀ nanocage: A theoretical investigation. Materials Research Express 5 (2018) 035006.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

16. **Saeedeh Kamalinahad**, Francesc Viñes, and Pablo Gamallo. Grazynes: Carbon-Based Two-Dimensional Composites with Anisotropic Properties. The journal of physical chemistry C 123 (2019) 27140-27149.

Type of production: Scientific paper

Format: Journal

Position of signature: 1

17. Motahareh Noormohammadbeigi, **Saeedeh Kamalinahad**, Farhad Izadi, Maryam Adimi and Alireza Ghasemkhani, Theoretical investigation of thioguanine isomers anticancer drug adsorption treatment on B₁₂N₁₂ nanocage. Materials Research Express 6 (2019) 1250g2.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

18. **Saeedeh Kamalinahad**, Azim Soltanabadi, Pablo Gamallo, B₃₆ bowl-like structure as nanocarrier for sulfonamides: a theoretical study. Monatshefte für Chemie-Chemical Monthly 151(2020)1785.

Type of production: Scientific paper

Format: Journal

Position of signature: 1

19. Motahareh Noormohammadbeigi, HamidReza Shamlouei, **Saeedeh Kamalinahad**, Alireza Ghasemkhani, Feasibility of Ca₁₂O₁₂ Nanocluster in Lithium and Sodium Atom/Ion Batteries: DFT Study. Journal of Inorganic and Organometallic Polymers and Materials 31(2021)1006

Type of production: Scientific paper

Format: Journal

Position of signature: 3

20. İnci SÖĞÜTLÜ, Sattar Arshadi, Evan Abdulkareem Mahmood, Vahideh Abbasi, **Saeedeh Kamalinahad**, Esmail Vessally, In silico investigation of metalophthalocyanine substituted in carbon nanocones (TM-PhCCNC, TM= Sc²⁺, Cr²⁺, Fe²⁺ and Zn²⁺) as a promising sensor for detecting N₂O gas involved in Covid-19. Journal of molecular structure, 1284 (2023) 135263.

Type of production: Scientific paper

Format: Journal

Position of signature: 5

21. Motahareh Noormohammadbeigi, **Saeedeh Kamalinahad**, Hamid Reza Shamlouei, Fatemeh Izadi Mehr, Raman Rajabi. In silico investigation of Al, Ga and Ge dopants effect on structural and electrical properties of pristine B₁₂N₁₂ nanocage toward acrolein adsorption. Journal of Inorganic and Organometallic Polymers and Materials. 33(2023) 3272-3281.

Type of production: Scientific paper

Format: Journal

Position of signature: 2

22. Saeedeh Kamalinahad, Esmail Vessally, Assessing the Sensing Performance of a Decorated B₂₂ Nanocluster for SO₂ Gas Detection: An In Silico Study. Journal of Sulfur Chemistry, Accepted (2023).

Type of production: Scientific paper

Format: Journal

Position of signature: 1

23. Faheem Abbas, Anupam Yadav, Karam Myaser Abd Alaziz, Maria Khalid, Nafis Ahmad, Michael M. Sabugaa, **Saeedeh Kamalinahad**, Exploring the Capabilities of Pristine B84 Nanocluster for Selective NO and N₂O Gases detection involved to COVID-19: A DFT analysis. Journal of Inorganic and Organometallic Polymers and Materials. Under revision.

24. **Saeedeh Kamalinahad**, Motahareh Noormohammadbeigi, Masoud Haratian, Pablo Gamallo, Felipe Fantuzzi, Aritra Roy. In silico investigation of Ca₁₂O₁₂ nanocage as hydrogen storage material. In preparation.

Type of production: Scientific paper

Format: Journal

Position of signature: 1

National and international conferences

1. Title of the work: New materials from computational simulations
Name of the conference: ANQUE -ICCE -CIBIQ
Geographical area: European Union
Type of participation: Participatory - oral communication
City of event: Santander, Spain
Date of event: 19/06/2019
2. Title of the work: Physisorption of toxic cyanogen gas onto exterior surface of pristine Al₁₂N₁₂ nanocluster: A theoretical study.
Name of the conference: 20th Iranian Physical chemistry Conference
Geographical area: Asian Union
Type of participation: Participatory - oral communication
City of event: Arak University- Arak/Iran
Date of event: 20/08/2017
3. Title of the work: Complexation of C₆₀ derivative as a carbonic anhydrase nanoscale enzyme inhibitor.
Name of the conference: 15th Iranian Physical chemistry Conference
Geographical area: Asian Union
Type of participation: Poster
City of event: Tehran University- Teharn/Iran
Date of event: 03/06/2012

4. Title of the work: Interaction energy and electronic structure details of complexes between some antiepileptic drugs and active site of CA enzyme.

Name of the conference: 15th Iranian chemistry Congress

Geographical area: Asian Union

Type of participation: Poster

City of event: Bu-Ali sina University- Hamedan/Iran

Date of event: 04/06/2011

Attended advanced, improvement and innovative teacher training

1. Title of course: SIESTA course
Organizing entity: Shahid Chamran Nanotechnology Research Center
Duration in hours: 21 hours
Start-End date: 17/09/2014 - 19/09/2014
2. Title of course: Introduction to QM/MM method
Organizing entity: Isfahan University of Technology
Duration in hours: 17 hours
Start-End date: 12/11/2014 - 13/11/2014
3. Title of course: Introduction to LAMMPS and VASP
Organizing entity: University de Barcelona
Duration in months: 6 months (During Sabbatical)
Start-End date: 09/2017 - 03/2018
4. Title of course: Introduction to Materials Studio
Organizing entity: Online workshop
Duration in hours: 10 hours
Start-End date: 03/2019 - 03/2019
5. Title of course: Introduction of Python
Organization entity: Online workshop
Duration in hours: 20 hours
Start-End date: 01/2020 -03/2020

Language

English Limited Working

Other activity

Description of the activity: Member of executive committee of 20th Iranian Physical Chemistry conference)

Organising entity: Arak University- Iranian Chemical society

Start-End date: 20/08/2017 - 22/08/2017

Awards

Elected student

1. Awarding entity: Payam Noor University of Arak
Date: 12/2006 & 12/2007
2. Awarding entity: Payam Noor University of Iran
Date: 03/2008
3. Awarding entity: Arak University
Date: 12/2016 & 12/2017
4. Selected student of National Elite Foundation
Date: 2016 & 2017

Top researcher

1. Awarding entity: Alzahra University
Date: 12/2013
2. Awarding entity: Committee of Research Week in Markazi Province / Arak University
Date: 12/2017