

# Hamidreza Ali Jouypazadeh

## Research Institute of Physics

Computational Materials Science Laboratory

Junior Researcher

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## Education

<b>Institution</b>	Arak University
<b>Faculty</b>	Faculty of Science/Department of Chemistry
<b>Date</b>	2012 - 2016
<b>Degree name</b>	PhD student

<b>Institution</b>	Shahid Beheshti University
<b>Faculty</b>	Faculty of Science/Department of Chemistry
<b>Date</b>	2009 - 2012
<b>Degree name</b>	Masters

<b>Institution</b>	Arak University
<b>Faculty</b>	Faculty of Science/Department of Chemistry
<b>Date</b>	2004 - 2009
<b>Degree name</b>	Bachelor

## Scientific Rank/degree

<b>Institution</b>	Arak University
<b>Date</b>	2016
<b>Degree name</b>	Candidate
<b>Specialty</b>	Chemical sciences
<b>Scientific Supervisor</b>	Prof. Mohammad Solimannejad
<b>Research Topic</b>	Ab initio intermolecular potential energy surfaces for complexes pairing linear molecules with rare gases

## Language skills

English یراف

## Work experience

<b>Institution</b>	Yerevan State University
<b>Period of time</b>	2025 till now

Rank/degree	Junior Researcher
Institution	Isfahan University of Technology
Period of time	2021 - 2024
Rank/degree	researcher
Institution	Isfahan University of Technology
Period of time	2018 - 2021
Rank/degree	Postdoc Researcher
Institution	Isfahan University of Technology
Period of time	2016 - 2018
Rank/degree	Research Assistant

## Publications

*Article*

**Enhancing ZnO monolayer nanosheets for photocatalysis: the role of FeSn and RuSn (n = 0-3) doping in electronic and structural properties**

Hamidreza Jouypazadeh, Esmail Vessally

New Journal of Chemistry 2024 13557-13565

*Article*

**Improving Photocatalytic activity of (100) and (111) TiO<sub>2</sub> nanosheets by coupling with ZrO<sub>2</sub> and HfO<sub>2</sub> nanosheets; A DFT-U study**

Suzan Mohammadi, Mohammadreza Mozdianfard, Hamidreza Jouypazadeh,

Mohammad Es'hagh-Davatgar

Journal of Physics and Chemistry of Solids 2024 111952

*Article*

**The Effect of Doping TiO<sub>2</sub> Monolayer with Sn<sup>+4</sup>, Pb<sup>+4</sup>, and S<sup>-2</sup> Ions on H<sub>2</sub> Production by Photocatalytic Water Splitting: Periodic DFT Modeling**

Nasim Orangi, Hossein Farrokhpour, Hamidreza Jouypazadeh, Fahimeh Eshaghzadeh

Iranian Journal of Science 2024 1351-1364

*Article*

**The adsorption of sulfur mustard chemical warfare agent on the Ga<sub>12</sub>N<sub>12</sub> and Ca<sub>12</sub>O<sub>12</sub> nanocages; A systematic DFT study**

Hamidreza Jouypazadeh, Hossein Farrokhpour, Esmail Vessally

Computational and Theoretical Chemistry 2023 114358

*Article*

**Theoretical study of the mechanism of Te (g) + 3F<sub>2</sub> (g)→TeF<sub>6</sub> (g)**

Fatemeh Hosseini, Hassan Hadadzadeh, Hossein Farrokhpour, Hamidreza Jouypazadeh

Molecular Physics 2022 e2059411

*Article*

**Be<sub>2</sub>C monolayer as an efficient adsorbent of toxic volatile organic compounds: theoretical investigation**

Hossein Farrokhpour, Mehrdad Gerami, Hamidreza Jouypazadeh

Molecular Physics 2022 e2132184,14

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*Article*

**Water-vapochromic behavior of a mononuclear Pd(II) complex of piroxicam: A DFT and TD-DFT study**

Hamidreza Jouypazadeh, Hossein Farrokhpour, Maedeh Karbasizadeh, Hassan Hadadzadeh

Journal of Molecular Graphics and Modelling 2021 107773

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*Article*

**Theoretical investigation of the water splitting photocatalytic properties of pristine, Nb and V doped, and Nb-V co-doped (1 1 1) TaON nanosheets**

Hamidreza Jouypazadeh, Hossein Farrokhpour, Mohamad Mohsen Momeni

Applied Surface Science 2021 148572

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*Article*

**Theoretical study of the vapochromic properties of a mononuclear Pd(II) complex with piroxicam ligands for the detection of the vapor of several solvents**

Hossein Farrokhpour, Hamidreza Jouypazadeh, Maedeh Karbasizadeh

Journal of Molecular Liquids 2021 116508

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*Article*

**Pd/Cu-Free Cobalt-Catalyzed Suzuki and Heck Using Green Bio-Magnetic Hybrid and DFT-Based Theoretical Study**

Abdol R. Hajipour, Zahra Khorsandi, Mehnoosh Ahmadi, Hamidreza Jouypazadeh, Bahareh Mohammadi,

Hossein Farrokhpour

Catalysis Letters 2021 2842–2850

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*Article*

**A DFT study of the water-splitting photocatalytic properties of pristine, Nb-doped, and V-doped Ta<sub>3</sub>N<sub>5</sub> monolayer nanosheets**

Hamidreza Jouypazadeh, Hossein Farrokhpour,, Mohamad Mohsen Momeni

Surfaces and Interfaces 2021 101379

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*Article*

**Interaction of different types of nanocages (Al<sub>12</sub>N<sub>12</sub>, Al<sub>12</sub>P<sub>12</sub>, B<sub>12</sub>N<sub>12</sub>, Be<sub>12</sub>O<sub>12</sub>, Mg<sub>12</sub>O<sub>12</sub>, Si<sub>12</sub>C<sub>12</sub> and C<sub>24</sub>) with HCN and ClCN: DFT, TD-DFT, QTAIM, and NBO calculations**

Hossein Farrokhpour, Hamidreza Jouypazadeh, Shirin Vakili Sohroforouzani

Molecular Physics 2020 1626506

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*Article*

**The Role of Delocalization Energy on Superhalogen Property: The Electron Affinity of**

Dr. Hossein Farrokhpour, Mostafa Yousefvand, Dr. Hassan Hadadzadeh, Dr. Hamidreza Jouypazadeh

ChemistrySelect 2020 3859-3873

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*Article*

**Theoretical insights into the electron affinity of manganese superhalogen compounds; NBO, QTAIM and energy decomposition analysis**

H. Farrokhpour, M. Yousefvand, H. Hadadzadeh, H. Jouypazadeh

Molecular Physics 2020 1718791

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*Article*

**Electron affinities of X12O12 (X = Be, Mg, and Ca), X12N12 (X = B, Al, and Ga), and X12P12 (X = B, Al, and Ga) nanocages: NBO calculations and energy decomposition analysis**

H. Farrokhpour, M. Yousefvand, H. Jouypazadeh, H. Hadadzadeh

European Physical Journal Plus 2020 719

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