# Hayk Ashot Zakaryan

hayk.zakaryan@ysu.am

**Research Institute of Physics**
Computational Materials Science Laboratory
Head of laboratory

## Education

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| **Institution** | Yerevan State University |
| **Faculty** | Radiophysics |
| **Date** | 2014 - 2017 |
| **Degree name** | PhD student |

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| **Institution** | Yerevan State University |
| **Faculty** | Radiophysics |
| **Date** | 2012 - 2014 |
| **Degree name** | Masters |

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| **Institution** | Yerevan State University |
| **Faculty** | Radiophysics |
| **Date** | 2008 - 2012 |
| **Degree name** | Bachelor |

## Scientific Rank/degree

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| **Institution** | Yerevan State University |
| **Date** | 2017 |
| **Degree name** | Candidate |
| **Specialty** | Physico-mathematical sciences |
| **Scientific Supervisor** | Vladimir Aroutiounian |
| **Research Topic** | Investigation of gas adsorption on the tin dioxide surface using density functional theory |

## Language skills

Հայերեն English Русский

## Publications

*Article*

**Material hardness descriptor derived by symbolic regression**
Hayk A. Zakaryan, Christian Tantardini, Zhong-Kang Han, Tariq Altalhi, Sergey V. Levchenko,

Alexander G. Kvashnin, Boris I. Yakobson

Journal of Computational Science 2024 102402

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*Article*

**Gas sensing properties of two dimensional tin oxides: A DFT study**
Areg Hunanyan, Nane Petrosyan, Hayk Zakaryan

Applied Surface Science 2024 160814

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*Article*

**Synthesis and evaluation of new mono- and binuclear salen complexes for the Cα-alkylation reaction of amino acid substrates as chiral phase transfer catalysts**
Anahit M. Hovhannisyan, Anna S. Tovmasyan, Anna F. Mkrtchyan, Karapet R. Ghazaryan,

Ela V. Minasyan, Olgert L. Dallakyan, Mikayel S. Chobanyan, Hayk Zakaryan, Giovanni N. Roviello,

Ashot S. Saghyan

Molecular Catalysis 2024 114618

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*Article*

**Computational Search and Stability Analysis of Two-Dimensional Tin Oxides**
Areg A. Hunanyan, Vladimir M. Aroutiounian, Hayk A. Zakaryan

Journal of Physical Chemistry C 2022 4647-4654

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*Article*

**Computational Design of Gas Sensors Based on V3S4 Monolayer**
Hayk A. Zakaryan, Misha A. Aghamalyan, Yevgeni Sh. Mamasakhlisov, Ilya V. Chepkasov,

Ekaterina V. Sukhanova, Alexander G. Kvashnin, Anton M. Manakhov, Zakhar I Popov,

Dmitry G. Kvashnin

Nanomaterials 2022 774

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*Article*

**2D-Mo3S4 phase as promising contact for MoS2**
H.A. Zakaryan, M.A. Aghamalyan, E.V. Sukhanova, A.G. Kvashnin, L.A. Bereznikova, D.G. Kvashnin,

Z.I. Popov

Applied Surface Science 2022 152971

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*Article*

**Adsorption of Hydrogen Peroxide on Two-Dimensional Transition Metal Chalcogenides**
M. A. Aghamalyan, V. M. Aroutiounian, E. S. Mamasakhlisov, E. V. Sukhanova, A. G. Kvashnin, Z. I. Popov,

A. A. Zakaryan

Journal of Contemporary Physics (Armenian Academy of Sciences) 2022 170-173

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*Article*

**Map of Two-Dimensional Tungsten Chalcogenide Compounds (W–S, W–Se, W–Te) Based on USPEX Evolutionary Search**
E. V. Sukhanova, A. G. Kvashnin, M. A. Agamalyan, H. A. Zakaryan, Z. I. Popov

JETP Letters 2022 292-296

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*Article*

**Computational Search and Stability Analysis of Two-Dimensional Tin Oxides**
Areg A. Hunanyan, Hayk A. Zakaryan, Vladimir M. Aroutiounian

Journal of Physical Chemistry C 2022 4647–4654

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*Article*

**Influence of UV Rays on the Volt-Capacity Characteristic of SnO2:Co Sensor of Vapors of Hydrogen Peroxide**

M. S. Aleksanyan, A. G. Sayunts, A. A. Zakaryan, V. M. Aroutiounian, V. M. Arakelyan, G. E. Shakhnazary

Journal of Contemporary Physics (Armenian Academy of Sciences) 2020 151-156

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*Article*

**Investigations of Sensors for Detection of Hydrogen Peroxide Vapors under the Influence of UV Illumination**

M. S. Aleksanyan, A. G. Sayunts, A. A. Zakaryan, V. M. Harutyunyan, V. M. Arakelyan,

G. E. Shakhnazaryan

Journal of Contemporary Physics (Armenian Academy of Sciences) 2020 205-212

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*Article*

**First-Principles Study of the Interaction of H2O2 with the SnO2 (110) Surface**

M. A. Aghamalyan, A. A. Hunanyan, V. M. Aroutiounian, M. S. Aleksanyan, A. G. Sayunts, H. A. Zakaryan

Journal of Contemporary Physics (Armenian Academy of Sciences) 2020 235-239

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*Article*

**Computational Search for New W−Mo−B Compounds**

Hayk A. Zakaryan, Alexander G. Kvashnin, Christian Tantardini, Yulia A. Kvashnina, Artem R. Oganov

Chemistry of Materials 2020 7028–7035

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*Article*

**ВЛИЯНИЕ УЛЬТРАФИОЛЕТОВЫХ ЛУЧЕЙ НА ВОЛЬТ- ЕМКОСТНУЮ ХАРАКТЕРИСТИКУ SnO2:Co СЕНСОРА ПАРОВ ПЕРЕКИСИ ВОДОРОДА**

М.С. АЛЕКСАНЯН, А.Г. САЮНЦ, А.А. ЗАКАРЯН, В.М. АРУТЮНЯН, В.М. АРАКЕЛЯН, Г.Э. ШАХНАЗАРЯН

Известия НАН РА. Физика (Journal of Contemporary Physics (Armenian Academy of Sciences) 2020

218-227

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*Article*

**ИССЛЕДОВАНИЕ СЕНСОРА ДЛЯ ОБНАРУЖЕНИЯ ПАРОВ ПЕРЕКИСИ ВОДОРОДА ПОД ДЕЙСТВИЕМ УЛЬТРАФИОЛЕТОВОГО ИЗЛУЧЕНИЯ**

М.С. АЛЕКСАНЯН, А.Г. САЮНЦ, А.А. ЗАКАРЯН, В.М. АРУТЮНЯН, В.М. АРАКЕЛЯН, Г.Э. ШАХНАЗАРЯН

Известия НАН РА. Физика (Journal of Contemporary Physics (Armenian Academy of Sciences) 2020

312-324

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*Article*

**Effects of UV Irradiation on the Sensing Properties of Co-doped SnO2 Thin Film for Ethanol Detection**

Mikayel Aleksanyan, Artak Sayunts, Hayk Zakaryan, Vladimir Aroutiounian, Gohar Shahnazaryan,

Valeri Arakelyan

International Journal on Advances in Systems and Measurements 2020 312-321

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*Article*

**Stable and hard hafnium borides: A first-principles study**

Congwei Xie, Qi Zhang, Hayk A. Zakaryan, Hao Wan, Ning Liu, Alexander G. Kvashni, Artem R.Oganov

Journal of Applied Physics 2019 205109(1-9)

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*Article*

**Formation Energy of Intrinsic and Impurity Defects in Tin Dioxide**
A. A. Hunanyan, M. A. Aghamalyan, V. M. Aroutiounian, H. A. Zakaryan

Journal of Contemporary Physics (Armenian Academy of Sciences) 2019 282–286

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*Article*

**New Tungsten Borides, their Stability and Outstanding Mechanical Properties**
Hayk A. Zakaryan, Alexander G. Kvashnin, Changming Zhao, Yifeng Duan, Yulia A. Kvashnina,

Congwei Xie, Huafeng Dong, Artem R Oganov

Journal of Physical Chemistry Letters 2018 3470–3477

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*Article*

**CO gas adsorption on SnO2 surfaces: density functional theory study**
Hayk Zakaryan, Vladimir Aroutiounian

Sensors & Transducers 2017 50-56

http://www.sensorsportal.com/HTML/DIGEST/Submission.htm

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*Article*

**Исследование структуры и дефектов легированного кобальтом диоксида олова: теория функциональной плотности и эмпирические силовые потенциалы**
А. А. Закарян, В. М. Арутюнян

Известия НАН РА. Физика (Journal of Contemporary Physics (Armenian Academy of Sciences) 2017

312-320

http://www.flib.sci.am/eng/Fizika/Frame.html

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*Article*

**Adsorption of CO gas molecules on SnO2 surface**
V.M. Aroutiounian, H.A. Zakaryan

International Scientific Journal for Alternative Energy and Ecology 2017 91-99

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*Article*

**ADSORPTION OF CO MOLECULES ON SNO 2 (110), (100), (101), (001) SURFACE ORIENTATIONS: DENSITY FUNCTIONAL THEORY STUDY**

H. Zakaryan

SEMICONDUCTOR MICRO- AND NANOELECTRONICS. PROCEEDINGS OF THE ELEVENTH INTERNATIONAL CONFERENCE
2017 88-91

http://icsmn.ysu.am/11th%20ICSMN-Proceedings.pdf

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*Article*

**Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO2**
Hayk A. Zakaryan, Alexander G. Kvashnin, Artem R. Oganov

Scientific Reports 2017 1 - 9

https://www.nature.com/articles/s41598-017-10331-z

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*Article*

**Adsorption of the H and H 2 O on SnO 2 Surfaces in an O 2 Environment: Density Functional Theory Study**

H. Zakaryan

Armenian Journal of Physics 2016 283-293

http://ajp.asj-oa.am/

*Article*

**Влияние влажности на запрещенную зону графена**

А.А.Закарян, В.М. Арутюнян

Известия НАН РА. Физика (Journal of Contemporary Physics (Armenian Academy of Sciences) 2015

350-356

http://www.flib.sci.am/eng/Fizika/Frame.html

*Conference*

**Ab initio investigation of CO gas sensing mechanism on SnO2 surfaces**

H. A. Zakaryan, V. M. Aroutiounian

*Conference*

**Cobalt impurity in thin dioxide and its influence in hydrogen sensors**

H. Zakaryan, V. Aroutiounian, M. Aghamalyan

*Conference*

**UV-assisted Chemiresistive Alcohol Sensor Based on Cobalt Doped Tin Dioxide**

Mikayel Aleksanyan, Artak Sayunts, Hayk Zakaryan, Vladimir Aroutiounian, Valeri Arakelyan,

Gohar Shahnazaryan