

# Hayk Ashot Zakaryan

✉ hayk.zakaryan@ysu.am



## Research Institute of Physics

Computational Materials Science Laboratory

Head of laboratory

## Education

---

<b>Institution</b>	Yerevan State University
<b>Faculty</b>	Radiophysics
<b>Date</b>	2014 - 2017
<b>Degree name</b>	PhD student

---

<b>Institution</b>	Yerevan State University
<b>Faculty</b>	Radiophysics
<b>Date</b>	2012 - 2014
<b>Degree name</b>	Masters

---

<b>Institution</b>	Yerevan State University
<b>Faculty</b>	Radiophysics
<b>Date</b>	2008 - 2012
<b>Degree name</b>	Bachelor

---

## Scientific Rank/degree

---

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

---

## Language skills

---

Հայերեն English Русский

---

## Publications

*Article*

### **Computational Search and Stability Analysis of Two-Dimensional Tin Oxides**

Areg A. Hunanyan, Vladimir M. Aroutiounian, Hayk A. Zakaryan

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

---

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

---

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

---

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. Aghamalyan, H. A. Zakaryan, Z. I. Popov

JETP Letters 2022 292-296

---

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

---

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

---

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

---

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

---

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

---

Article

**ВЛИЯНИЕ УЛЬТРАФИОЛЕТОВЫХ ЛУЧЕЙ НА ВОЛЬТ- ЕМКОСТНУЮ ХАРАКТЕРИСТИКУ SnO<sub>2</sub>:Co СЕНСОРА ПАРОВ ПЕРЕКИСИ ВОДОРОДА**

М.С. АЛЕКСАНИЯН, 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

---

Article

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

М.С. АЛЕКСАНИЯН, 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

---

Article

**Effects of UV Irradiation on the Sensing Properties of Co-doped SnO<sub>2</sub> 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

---

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)

---

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

---

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

---

Article

**CO gas adsorption on SnO<sub>2</sub> surfaces: density functional theory study**

Hayk Zakaryan, Vladimir Aroutiounian

Sensors & Transducers 2017 50-56

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

---

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>

---

*Article*

**Adsorption of CO gas molecules on SnO<sub>2</sub> surface**

V.M. Aroutiounian, H.A. Zakaryan

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

---

*Article*

**ADSORPTION OF CO MOLECULES ON SnO<sub>2</sub> (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.yasu.am/11th%20ICSMN-Proceedings.pdf>

---

*Article*

**Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO<sub>2</sub>**

Hayk A. Zakaryan, Alexander G. Kvashnin, Artem R. Oganov

Scientific Reports 2017 1 - 9

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

---

*Article*

**Adsorption of the H and H<sub>2</sub>O on SnO<sub>2</sub> Surfaces in an O<sub>2</sub> 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 SnO<sub>2</sub> 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

---