

# Айк Ашот Захарян

✉ hayk.zakaryan@ysu.am



## Научно-исследовательский институт физики

Հաշվարկային նյութագիտության լաբորատորիա  
Заведующий лабораторией

## Образование

Учреждение	Ереванский Государственный Университет
Факультет	Радиофизика
Дата	2014 - 2017
Степень / Звание	Аспирант

Учреждение	Ереванский Государственный Университет
Факультет	Радиофизика
Дата	2012 - 2014
Степень / Звание	Магистр

Учреждение	Ереванский Государственный Университет
Факультет	Радиофизика
Дата	2008 - 2012
Степень / Звание	Бакалавр

## Ученое звание/Ученая степень

Учреждение	Ереванский Государственный Университет
Дата	2017
Степень / Звание	Кандидат наук
Специальность	Физико-математические науки
Научный руководитель	Владимир Арутюнян
Научная тема	Исследование адсорбции газов на поверхности диоксида олова с помощью теории функционала плотности

## Знание языков

Հայերեն English Русский

## Публикации

Статья

### Computational screening for novel solid-state electrolytes in Li3MX6 composition

Hayk A. Zakaryan, Olgert L. Dallakyan, Alexey P. Maltsev, Ilya V. Chepkasov, Misha A. Aghamalyan,

Areg A. Hunanyan, Nane Z. Petrosyan, Mikayel S. Chobanyan, Mikayel T. Sahakyan,  
Luiza G. Khachatryan, Artem R. Oganov  
Journal of Energy Chemistry 2026 495-504

---

Статья

**Glaser Heterocoupling Reaction for the Synthesis of Enantiomerically Enriched Unnatural  $\alpha$ -Amino Acids Incorporating Asymmetric Diyne Moieties: Mechanistic Insights and Optimization**

Liana Hayriyan, Anna Tovmasyan, Anna Grigoryan, Karapet Ghazaryan, Barbara Biondi,

Olgert L. Dallakyan, Mikayel S. Chobanyan, Hayk Zaqaryan, Ashot Saghyan, Anna Mkrtchyan

ACS Omega 2025 A-G

---

Статья

**A DFT study on an 18-crown-6-like-N8 structure as a material for metal ion storage: stability and performance**

Hayk Zakaryan, Irina I. Piyanzina, Sadegh Kaviani, Regina M. Burganova, Oleg V. Nedopekin

Sustainable Energy and Fuels 2025 5075-5084

---

Статья

**DFT analysis of furan-based covalent organic framework as electrode materials for lithium and calcium ion batteries**

Irina Piyanzina, Aigul Shamsieva, Alexander Evseev, Sadegh Kaviani, Oleg Nedopekin, Hayk Zakaryan

Computational and Theoretical Chemistry 2025 115445

---

Статья

**Accelerated composition optimization of hybrid perovskites via data-driven materials design, DFT calculations and synthesis**

Sona Grigoryan, Nane Petrosyan, Gurgen Kolotyan, Arpine Kozmalyan, Varazdat Avetisyan,

Hayk Zakaryan, Michael J. Schöning, Arevik Asatryan, Hayk Khachatryan

Materials and Design 2025 114902

---

Статья

**DFT investigation of magnetocrystalline anisotropy in Fe, Co, Pd<sub>0.97</sub>Co<sub>0.03</sub> and Pd<sub>0.97</sub>Fe<sub>0.03</sub> systems: from bulk to thin-films**

Irina I. Piyanzina, Regina M. Burganova, Hayk Zakaryan, Zarina I. Minnegulova, Igor V. Yanilkin,

Amir I. Gumarov

European Physical Journal Plus 2025 949

---

Статья

**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

---

Статья

**Gas sensing properties of two dimensional tin oxides: A DFT study**

Areg Hunanyan, Nane Petrosyan, Hayk Zakaryan

Applied Surface Science 2024 160814

---

Статья

**Synthesis and evaluation of new mono- and binuclear salen complexes for the  $\alpha$ -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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**Influence of UV Rays on the Volt-Capacity Characteristic of SnO<sub>2</sub>: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

---

*Статья*

**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

---

*Статья*

**First-Principles Study of the Interaction of H<sub>2</sub>O<sub>2</sub> with the SnO<sub>2</sub> (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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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)

---

*Статья*

**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

---

*Статья*

**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

---

*Статья*

**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>

---

*Статья*

**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>

---

*Статья*

**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

---

*Статья*

**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>

---

*Статья*

**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>

---

*Статья*

**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/>

---

*Статья*

**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

*Конференция*

**Ab initio investigation of CO gas sensing mechanism on SnO<sub>2</sub> surfaces**

H. A. Zakaryan, V. M. Aroutiounian

---

*Конференция*

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

H. Zakaryan, V. Aroutiounian, M. Aghamalyan

---

*Конференция*

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

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

Gohar Shahnazaryan

---