Hayk Ashot Zakaryan

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Նյութագիտության և նանոտեխնոլոգիաների գիտական կենտրոն
Հաշվարկային նյութագիտության լաբորատորիա
head of laboratory

Research Institute of Physics
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head of laboratory

Institute of Physics
Chair of Materials Science and Nanotechnology
Assistant

Education

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

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

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

Scientific Rank/degree

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

Language skills

Publications

Article

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

Article

Towards structure-property prediction in DyF3 nanoclusters
Regina M. Burganova, Zafari Umar, Ilya V. Chepkasov, Hayk Zakaryan, Irina I. Piyanzina

Computational and Theoretical Chemistry 2026 115657

https://www.sciencedirect.com/science/article/pii/S2210271X26000010?via%3Dihub

Article

Computational Discovery of Li6PO5I: An Oxide Argyrodite for Solid-State Electrolytes
Nane Petrosyan, Areg Hunanyan, Olgert Dallakyan, Luiza Khachatryan, Mikayel Sahakyan,

Mikayel Chobanyan, Hayk Zakaryan

ACS Applied Energy Materials 2026 1159–1167

https://pubs.acs.org/doi/10.1021/acsaem.5c03545

Article

Dielectric function of layered GaSe0.8Te0.2 and emergent all van der Waals optical elements
A. V. Margaryan, M. L. Sargsyan, I. I. Piyanzina, D. A. Karakhanyan, M. H. Hayrapetyan, M. A. Levonyan,

H. A. Zakaryan, K. S. Novoselov, D. A. Ghazaryan

Scientific Reports 2026 12551

https://doi.org/10.1038/s41598-026-42182-y

Article

Machine-learning-accelerated discovery of amorphous lithium-ion electrolytes
Areg Hunanyan, Hayk Zakaryan

Computational Materials Science 2026 114732

https://doi.org/10.1016/j.commatsci.2026.114732

Article

Glaser Heterocoupling Reaction for the Synthesis of Enantiomerically Enriched Unnatural α-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

Article

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

Article

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 & Fuels 2025 5075-5084

Article

DFT investigation of magnetocrystalline anisotropy in Fe, Co, Pd0.97Co0.03 and Pd0.97Fe0.03 systems: from bulk to thin-films

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

Amir I. Gumarov

The European Physical Journal Plus 2025 949

Article

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

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

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

Materials & Design 2025 114902

Article

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

Areg Hunanyan, Nane Petrosyan, Hayk Zakaryan

Applied Surface Science 2024 160814

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

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

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. Agamalyan, 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

The 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

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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

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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

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 SnO2:Co СЕНСОРА ПАРОВ ПЕРЕКИСИ ВОДОРОДА
М.С. АЛЕКСАНЯН, А.Г. САЮНЦ, А.А. ЗАКАРЯН, В.М. АРУТЮНЯН, В.М. АРАКЕЛЯН, Г.Э. ШАХНАЗАРЯН

Proceedings of NAS RA Physics 2020 218-227

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

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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

Conference

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

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

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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

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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

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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

The Journal of Physical Chemistry Letters 2018 3470–3477

Conference

Cobalt impurity in thin dioxide and its influence in hydrogen sensors

H. Zakaryan, V. Aroutiounian, M. Aghamalyan

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Article

CO gas adsorption on SnO2 surfaces: density functional theory study

Hayk Zakaryan, Vladimir Aroutiounian

Sensors & Transducers 2017 50-56

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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

Proceedings of NAS RA Physics 2017 312-320

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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

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
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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

Conference

Ab initio investigation of CO gas sensing mechanism on SnO2 surfaces
H. A. Zakaryan, V. M. Aroutiounian

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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

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Article

Влияние влажности на запрещенную зону графена
А.А.Закарян, В.М. Арутюнян

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