

Hayk Ashot Zakaryan

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Research Institute of Physics

Computational Materials Science Laboratory

Head of laboratory

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
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

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

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

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

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

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

Article

DFT investigation of magnetocrystalline anisotropy in Fe, Co, Pd_{0.97}Co_{0.03} and Pd_{0.97}Fe_{0.03} 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

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

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

Areg Hunanyan, Nane Petrosyan, Hayk Zakaryan
Applied Surface Science 2024 160814

Article

Synthesis and evaluation of new mono- and binuclear salen complexes for the α -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 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

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

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 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

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

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

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 SnO₂ 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 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 SNO₂ (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 RuO₂

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 H₂O on SnO₂ Surfaces in an O₂ 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

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
