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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 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

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_{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

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 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

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 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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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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Статья

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

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 SnO₂: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 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

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)

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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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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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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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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

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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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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>

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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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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/>

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 SnO₂ 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
