

Hayk Zakaryan



Date of Birth: December 28, 1991
Citizenship: Republic of Armenia
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ORCID ID: [0000-0002-6105-3013](https://orcid.org/0000-0002-6105-3013)
Researcher ID: [F-2103-2017](https://orcid.org/F-2103-2017)
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Work Experience: **2022-present Yerevan State University**

Head of Computational Materials Science Laboratory of Center of Semiconductor devices and Nanotechnology

2018 – present

Committee member of “Young Scientist Support Program”, The RA Ministry of Education, Science, Culture and Sports

2017-2021 present Yerevan State University

Research scientist

Faculty: Physics of Semiconductors and Microelectronics

Center of Semiconductor devices and Nanotechnology

Skolkovo Institute of Science and Technology

Feb., 2016 - August, 2016

Junior Researcher

Center of Design, Manufacturing and Materials

Lab: Computational materials and design

Memoir Systems Yerevan Branch.

September, 2012 - March, 2015

Hardware Engineer

Institute of Applied Problems of Physics, Academy of Sciences of the Republic of Armenia

September 1, 2009 - January 29, 2010

Laboratory assistant in the department of repair

Education: **2014-2017 Yerevan State University (PhD)**

Faculty: Physics of Semiconductors and Microelectronics

2012-2014 Yerevan State University (Master degree)

Department: Radiophysics
Faculty: Physics of Semiconductors and Microelectronics
Graduated with honors
2008-2012 Yerevan State University (Bachelor degree)
Specialization: Radiophysics and Electronics
Graduated with honors
2006-2008 Specialized College "Quantum"
Major: physics and mathematics

Publications:

1. Zakaryan AA, Aroutiounian VM. Influence of humidity on the graphene band gap. *J Contemp Phys (Armenian Acad Sci)*. 2015;50(3):263-267. doi:10.3103/s106833721503007x
2. Zakaryan H. Adsorption of the H and H₂O on SnO₂ Surfaces in an O₂ Environment: Density Functional Theory Study. *Armen J Phys*. 2016;9(4):283-293.
3. Zakaryan HA, Kvashnin AG, Oganov AR. Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO₂. *Sci Rep*. 2017;7(1):10357. doi:10.1038/s41598-017-10331-z
4. Zakaryan H, Aroutiounian V. Investigation of cobalt doped tin dioxide structure and defects: Density functional theory and empirical force fields. *J Contemp Phys (Armen Acad Sci)*. 2017;52(3):227-233. doi:10.3103/S1068337217030070
5. Kvashnin AG, Zakaryan HA, Zhao C, et al. New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. *J Phys Chem Lett*. 2018;9(12):3470-3477. doi:10.1021/acs.jpcclett.8b01262
6. Hunanyan AA, Aghamalyan MA, Aroutiounian VM, Zakaryan HA. Formation Energy of Intrinsic and Impurity Defects in Tin Dioxide. *J Contemp Phys (Armen Acad Sci)*. 2019;54(3):282-286. doi:10.3103/S1068337219030083
7. Xie C, Zhang Q, Zakaryan HA, et al. Stable and hard hafnium borides: A first-principles study. *J Appl Phys*. 2019;125(20):205109. doi:10.1063/1.5092370
8. Aleksanyan MS, Sayunts AG, Zakaryan AA, Aroutiounian VM, Arakelyan VM, Shakhnazaryan GE. Influence of UV Rays on the Volt-Capacity Characteristic of SnO₂:Co Sensor of Vapors of Hydrogen Peroxide. *J Contemp Phys*. 2020;55(2):151-156. doi:10.3103/S1068337220020048
9. Aleksanyan MS, Sayunts AG, Zakaryan AA, Harutyunyan VM. Investigations of Sensors for Detection of Hydrogen Peroxide Vapors under the Influence of UV Illumination. *J Contemp Phys (Armen Acad Sci)*. 2020;55(3):205-212. doi:10.3103/S1068337220030032
10. Aghamalyan MA, Hunanyan AA, Aroutiounian VM, Aleksanyan MS, Sayunts AG, Zakaryan HA. First-Principles Study of the Interaction of H₂O₂ with the SnO₂ (110) Surface. *J Contemp Phys (Armen Acad Sci)*. 2020;55(3):235-239. doi:10.3103/S1068337220030020
11. Kvashnin A, Tantardini C, Zakaryan H, Kvashnina Y, Oganov A. Computational Search for New W–Mo–B Compounds. *Chem Mater*. 2020. doi:10.1021/acs.chemmater.0c02440
12. The Journal of Physical Chemistry C, 2022, 126 (9), 4647-4654, Areg A. Hunanyan, Vladimir M. Aroutiounian, Hayk A. Zakaryan - Computational Search and Stability Analysis of Two-Dimensional Tin Oxides
13. Nanomaterials, 2022, 12 (5), 774, Ilya V. Chepkasov, Ekaterina V. Sukhanova, Alexander G. Kvashnin, Hayk A. Zakaryan, Misha A. Aghamalyan, Yevgeni Sh. Mamasakhlisov, Anton M. Manakhov, Zakhar I. Popov, Dmitry G. Kvashnin - Computational Design of Gas Sensors Based on V₃S₄ Monolayer
14. Applied Surface Science, 2022, 589, 152971, E.V. Sukhanova, A.G. Kvashnin, L.A. Bereznikova, H.A. Zakaryan, M.A. Aghamalyan, D.G. Kvashnin, Z.I. Popov - 2D-Mo₃S₄ phase as promising contact for MoS₂
15. JETP Letters, 2022, 115 (5), 292-296, E. V. Sukhanova, A. G. Kvashnin, M. A. Agamalyan,

- H. A. Zakaryan, Z. I. Popov - Map of Two-Dimensional Tungsten Chalcogenide Compounds (W–S, W–Se, W–Te) Based on USPEX Evolutionary Search
16. Journal of Contemporary Physics (Armenian Academy of Sciences), 2022, 57 (2), 170-173,
M. A. Aghamalyan, V. M. Aroutiounian, E. Sh. Mamasakhlisov, E. V. Sukhanova, A. G. Kвашnin, Z. I. Popov, A. A. Zakaryan - Adsorption of Hydrogen Peroxide on Two-Dimensional Transition Metal Chalcogenides

Grants: 2023-2028, Computational materials design and discovery for energy storage applications, Science Committee RA, (PI)
2022-2023, High-Throughput Search for Novel Solid-State Electrolytes Using Machine-Learning, Faculty research funding, Enterprise Incubator Foundation (EIF) with support of PMI Science, (group head)
2021-2022, Computational search for novel solid-state electrolytes, Oracle for research grant, 16576595, (PI)
2021-2022, Computational Search for Novel Solid-State Electrolytes, ANSEF, EN-matsc-2660, (PI)
2020-2023, Computational search for novel solid state electrolytes, 20TTSG-2F010, Science Committee RA, (PI)
2021-2022, Search and investigation for novel two dimensional materials for biochemical sensing applications, 20RF-185, Science Committee RA-RF international grant, (member)
2019 Faculty research funding, Enterprise Incubator Foundation (EIF) with support of PMI Science, (group head)
2019 European Partnership (EaPEC 2019), (PI)
2019-2021, Scientific Committee of RA grant (19YR-2K002), (member)
2018-2020, RA-RF international grant (18RF-118), (member)
2017-2018 Russian Science Foundation project No 17-73-20038, (member)
2014 – 2017, NATO project Sfp-984597, (member)

Conferences: Conference and tutorial on Physics of Defects in Solids: Quantum Mechanics Meets Topology, Trieste, Italy, July, 2018.
ALLSENSORS 2017: “The Second International Conference on Advances in Sensors, Actuators, Metering and Sensing”, France, Nice, March 19-23, 2017.
H. A. Zakaryan and V. M. Aroutiounian, “Sensitivity of graphene humidity sensors,” in Proc. of SENSOR 2015 and IRS 2 2015, Nierenberg, Germany, 2015, pp. 868–872.
Conference on Frontiers of Nanoscience, ICTP (International Center for Theoretical Physics), Italy, Aug 23 – Sep1, 2015.

Workshops: Hands-on DFT and Beyond, Beijing, China, July 29 – August 14, 2018.
Combined Topological and DFT Methods for Prediction of New Materials II,

Workshop, Samara, Russia, July, 2016.

Nanoscience, ISU Kassel, Germany, June 20 – July 18, 2015.

Scholarships: Scholarship by University of Kassel for workshop, Germany, June 20 – July 18, 2015

Scholarship for PhD degree by Yerevan State University, 2014 -2017

Scholarship for study Master degree by Yerevan State University, 2012-2014

Scholarship for study Bachelor degree by Yerevan State University, 2008-2012

Technical Skills: VASP, USPEX, Quantum Espresso, Python

Languages: Russian (Excellent), English (Excellent), Armenian(native).

Interests and activities: Philosophy, astronomy, fiction, sport.