

# Zakar Khachik Papanyan

✉ z.papanyan@ysu.am



## Research Center for Chemistry

Ֆիզիկական քիմիայի լաբորատորիա

Researcher

## Education

---

<b>Institution</b>	Yerevan State University
<b>Faculty</b>	Faculty of chemistry
<b>Date</b>	2009 - 2011
<b>Degree name</b>	Masters

---

<b>Institution</b>	Yerevan State University
<b>Faculty</b>	Faculty of chemistry
<b>Date</b>	2005 - 2009
<b>Degree name</b>	Bachelor

## Scientific Rank/degree

---

<b>Institution</b>	Faculty of chemistry
<b>Date</b>	2014
<b>Degree name</b>	Candidate
<b>Specialty</b>	Chemical sciences
<b>Scientific Supervisor</b>	Sh. Markarian
<b>Research Topic</b>	Molecular interactions and chemical transformations of cysteine in the sulfoxide-water solutions

## Language skills

---

English Русский

## Work experience

---

<b>Institution</b>	Laboratory of physical chemistry at chemistry research center, YSU
<b>Period of time</b>	2014 till now
<b>Rank/degree</b>	resercher

## Scientific interests

---

- Molecular modelling and computational chemistry, methods of spectroscopy

---

## Publications

---

*Article*

**QUANTUM CHEMICAL CALCULATION OF STRUCTURAL AND THERMODYNAMIC PROPERTIES OF ETHYL METHYL SULFONE IN THE GAS PHASE**

L. S. Gabrielyan, Z. Kh. Papanyan

Proceedings of the YSU B: Chemical and Biological Sciences 2023 199-206

---

*Article*

**PREDICTION OF DIPROPYL SULFONE PROPERTIES BY DENSITY FUNCTIONAL THEORY METHODS: CONFORMATIONAL ANALYSIS AND SIMULATED IR SPECTRUM**

Z. Kh. PAPANYAN, L. S. GABRIELIAN

Proceedings of the YSU B: Chemical and Biological Sciences 2022 185-202

---

*Article*

**Volumetric, UV-Vis and FT IR Studies of Isoniazid in Diethylsulfoxide Solutions**

Shiraz A. Markarian, Zakar K. Papanyan, Gohar A. Shahinyan

Journal of Solution Chemistry 2020 1-13

---

*Article*

**Quantum chemical study on the solvation of lithium chloride in dimethyl- and diethyl sulfones**

A.S. Mkhitarian, Z. K. Papanyan, L.S. Gabrielyan

Proceedings of the YSU B: Chemical and Biological Sciences 2018 10-19

<http://www.y-su.am/science/hy/1520431333>

---

*Article*

**Theoretical ab initio calculation of entropy and heat capacity of dialkylsulfones in the gas phase**

A.S. Mkhitarian, Z.K. Papanyan, L.S. Gabrielyan, S.A. Markarian

Chemical Journal of Armenia 2018 13-22

---

*Article*

**КВАНТОВО-ХИМИЧЕСКОЕ ОПРЕДЕЛЕНИЕ ТЕПЛОТЫ ГИДРАТАЦИИ ДИЭТИЛСУЛЬФОНА**

Л.С. Габриелян, Ш.А. Маркарян, З.Х. Папаян, А.С. Мхитарян

Известия высших учебных заведений. Серия: химия и химическая технология (ChemChemTech) 2018 17-21

---

*Article*

**AB INITIO HARTREE-FOCK AND DENSITY FUNCTIONAL THEORY INVESTIGATIONS ON THE POTENTIAL ENERGY SURFACE AND VIBRATIONAL SPECTRA OF DIETHYL SULFONE**

Z. Kh. PAPANYAN, A. S. MKHITARYAN, L. S. GABRIELIAN

Proceedings of the YSU B: Chemical and Biological Sciences 2018 147-154

---

*Article*

**DETECTION OF OXIDATION OF L-CYSTEINE BY DIMETHYL SULFOXIDE IN AQUEOUS SOLUTIONS BY IR SPECTROSCOPY**

PAPANYAN Z., MARKARIAN S.

*Conference*

**AB INITIO STUDY OF LITHIUM CHLORIDE SOLVATION BY SULFONES**

Gabrielyan L.S., Mkhitarian A.S., Papanyan Z.K., Markarian S.A.

---

*Conference*

**Quantum Chemical Calculation of Thermodynamic Properties of Diethyl Sulfone**

Gabrielyan L.S., Papanyan Z.K., Mkhitarian A.S.

---

*Conference*

**UV-VIS AND THERMODYNAMIC STUDIES OF COMPLEX FORMATION OF DIETHYLSULFOXIDE WITH CoCl<sub>2</sub> AND NiCl<sub>2</sub>**

H.H. Ghazoyan, H.R. Sargsyan, Z.K. Papanyan, S.A. Markarian

---

*Conference*

**UV-VIS AND FT IR STUDY OF COMPLEX FORMATION BETWEEN ISONIAZID AND DIMETHYLSULFOXIDE OR DIETHYLSULFOXIDE**

G.A. Shahinyan, Z.K. Papanyan, S.A. Markarian

---

*Conference*

**COMPOSITION AND TEMPERATURE DEPENDENCE OF SURFACE TENSION AND DENSITY OF AQUEOUS SOLUTIONS OF DIBUTYL SULFONE**

Manucharyan V.K., Papanyan Z.K., Gabrielyan L.S.

---

*Conference*

**Quantum chemical studies of lithium ion/sulfone complexes**

Zakar Papanyan, Liana Gabrielyan

---

*Conference*

**CONFORMATIONAL AND VIBRATIONAL ANALYSIS OF DIPROPYL SULFONE BY DENSITY FUNCTIONAL THEORY METHODS**

Papanyan Z., Gabrielyan L.

---

*Conference*

**DFT AND EXPERIMENTAL UV/VIS SPECTRA OF SELECTED AZO DYES**

Petrosyan S., Papanyan Z., Zatikyan A., Gabrielyan L.

---