

# Irina Ivanovna Gumarova

## Research Institute of Physics

Computational Materials Science Laboratory

Researcher

✉ irina.gumarova@ysu.am



## Language skills

English

## Publications

*Article*

### **Phosphonic acid-functionalized g-C<sub>3</sub>N<sub>4</sub> nanosheets for chromium (Cr<sup>6+</sup>) adsorption from aqueous solutions: Experimental insights and density functional theory calculations**

Irina Piyanzina, Mohammad Khajavian, Dmitrii A. Tayurskii, Oleg V. Nedopekin, Vahid Vatanpour,

Suzylawati Ismail

Inorganic Chemistry Communications 2025 113971

*Article*

### **First-principles design of GaN-VHC (H = Cl, Br; C = Se, Te) van der Waals heterostructures for advanced optoelectronic applications**

Piyanzina Irina, Sheraz Ahmad, Shah Saleem Ullah, Haleem Ud Din, Cuong Q. Nguyen

RSC Advances 2025 13076-13085

*Article*

### **Magnetoelectric and spin-lattice effects in Fe/BaTiO<sub>3</sub> heterostructure: non-collinear DFT calculations**

Piyanzina I. I., Burganova R., Kamashev A. A., Mamin R. F.

Magnetic Resonance in Solids 2025 25203

*Article*

### **A DFT study on an 18-crown-6-like-N<sub>8</sub> 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*

### **Realization of Mn<sup>6+</sup>-NIR-II broadband emission in BaCrO<sub>4</sub> and its nanolization via liquid-solid method**

Irina I. Piyanzina, Linyun Zeng, Chunli Li, Wenjing Huang, Jiahui Zhang, Zafari Umar, Yuliya Bokshyts,

Bekhzodjon Abdurahmonovich Abdurakhimov, Peican Chen, Xinguo Zhang

Ceramics International 2025 33045-33055

*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

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*Article*

**Design and strain engineering of stable 2D TiSi<sub>2</sub>N<sub>4</sub> photocatalyst: first-principles insights into water splitting and visible-light absorption**

Irina Piyanzina, Sheraz Ahmad, Haleem Ud Din

Computational and Theoretical Chemistry 2025 115415

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*Article*

**DFT investigation of magnetocrystalline anisotropy in Fe, Co, Pd<sub>0.97</sub>Co<sub>0.03</sub> and Pd<sub>0.97</sub>Fe<sub>0.03</sub> 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

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