Irina Ivanovna Gumarova

irina.gumarova@ysu.am

Նյութագիտության և նանոտեխնոլոգիաների գիտական կենտրոն
Հաշվարկային նյութագիտության լաբորատորիա
Scientific Worker

Research Institute of Physics

Նյութագիտության և նանոտեխնոլոգիաների գիտական կենտրոն
Հաշվարկային նյութագիտության լաբորատորիա
Scientific Worker

Language skills

English

Publications

Article

Effect of 3d transition metal doping (Mn, Fe, Co, Ni) on the electronic and magnetic properties of Pd alloys at low impurity concentrations: An Ab initio study
Irina I. Piyanzina, Zarina I. Minnegulova, Regina M. Burganova, Oleg V. Nedopekin, Igor V. Yanilkin, Vasiliy S. Stolyarov, Amir I. Gumarov

Computational and Theoretical Chemistry 2026 115620

https://www.sciencedirect.com/science/article/pii/S2210271X25005560

Article

Towards structure-property prediction in DyF3 nanoclusters
Regina M. Burganova, Zafari Umar, Ilya V. Chepkasov, Hayk Zakaryan, Irina I. Piyanzina

Computational and Theoretical Chemistry 2026 115657

https://www.sciencedirect.com/science/article/pii/S2210271X26000010?via%3Dihub

Article

Dielectric function of layered GaSe0.8Te0.2 and emergent all van der Waals optical elements
A. V. Margaryan, M. L. Sargsyan, I. I. Piyanzina, D. A. Karakhanyan, M. H. Hayrapetyan, M. A. Levonyan, H. A. Zakaryan, K. S. Novoselov, D. A. Ghazaryan

Scientific Reports 2026 12551

https://doi.org/10.1038/s41598-026-42182-y

Article

Machine learning prediction of Hubbard parameter in the DFT+U approach
Ruslan Akhmerov, Oleg Nedopekin, Irina I. Piyanzina

Computational Condensed Matter 2026 e01275

https://doi.org/10.1016/j.cocom.2026.e01275

Article

First-principles computational design of a novel two-dimensional SHfSiN2 anode for lithium,

sodium, and multivalent metal ion batteries
Sheraz Ahmad, Nouari Saheb, Arifur Rahman, Irina Piyanzina

Journal of Power Sources 2026 240277

https://doi.org/10.1016/j.jpowsour.2026.240277

Article

Phosphonic acid-functionalized g-C3N4 nanosheets for chromium (Cr6+) 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/BaTiO3 heterostructure: non-collinear DFT calculations
Piyanzina I. I., Burganova R., Kamashev A. A., Mamin R. F.

Magnetic Resonance in Solids 2025 25203

Article

Realization of Mn6+NIR-II broadband emission in BaCrO4 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

Design and strain engineering of stable 2D $TiSi_2N_4$ photocatalyst: first-principles insights into water splitting and visible-light absorption
Irina Piyanzina, Sheraz Ahmad, Haleem Ud Din

Computational and Theoretical Chemistry 2025 115415

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

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 & Fuels 2025 5075-5084

Article

DFT investigation of magnetocrystalline anisotropy in Fe, Co, Pd0.97Co0.03 and Pd0.97Fe0.03 systems: from bulk to thin-films
Irina I. Piyanzina, Regina M. Burganova, Hayk Zakaryan, Zarina I. Minnegulova, Igor V. Yanilkin, Amir I. Gumarov
The European Physical Journal Plus 2025 949

Article

Site preference identification and crystal field analysis of high-efficient and thermal-stable NIR-I emission in NaAl11O17:Fe3+: experimental and DFT investigation
Irina I. Piyanzina, Chunli Li, Linyun Zeng, Ziyi Hong, Wenjia Xie, Peican Chen, Liya Zhou, Chunyan Zhou, Jialiang Pan, Wei Liu, Weitao Ren, Xinguo Zhang
Progress in Solid State Chemistry 2025 100551
https://www.sciencedirect.com/science/article/pii/S0079678625000445
