

RESULTS

Published articles

Ana Maria Toader, Bogdan Frecus, Corneliu I. Oprea, Maria Cristina Buta
Physchem 2023, 3, 270–289.

Alice Mischie, Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu
Computational and Theoretical Chemistry, 2023, 1230, 114370

Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu
Chemistry Journal of Moldova 2023, 18(2), 78-86

Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu, Adela Mihai
Symmetry 2024, 16, 22

Ana Maria Toader, Maria Cristina Buta, Werner Urland, Alessandro Stroppa, Fanica Cimpoesu
Computational Materials Science 2024, 235, 112742

H. Zheng, A. Ghosh, M. J. Swamynadhan, Q. Zhang, W. P. D. Wong, Z. Wu, R. Zhang, J. Chen, F. Cimpoesu, S. Ghosh, B. J. Campbell, K. Wang, A. Stroppa, R. Mahendiran, K. P. Loh
Nature Communications 2024, 15, 5556

Adela Mihai, Ion Mihai
International Electronic Journal of Geometry 2024, 17(1), 15–23

Stefan-Cezar Broscateanu, Adela Mihai, Andreea Olteanu
Symmetry 2024, 16, 1361

L. Pricop, G. Ionita, N. Stanica, C. Enachescu, R. Tanasa, M. Ferbinteanu
Journal of Coordination Chemistry, 2024, accepted;

Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu, and Marilena Ferbinteanu
ChemPlusChem 2024, accepted; DOI:10.1002/cplu.202400632

Under review articles

Fanica Cimpoesu, M. Cristina Buta, Ana M. Toader, Ionel Humelnicu, Werner Urland, Dumitru-Claudiu Sergentu, Markus Suta, Ab initio modelling of the photoluminescence of $\text{SrCl}_2\text{:Eu}^{2+}$ - Direct comparison between density functional and wavefunction theory-based approaches. Send to *Inorganic Chemistry*, Manuscript ID: ic-2024-05073b

Ana M. Toader, M. Cristina Buta, Werner Urland, Alessandro Stroppa, Fanica Cimpoesu, On the Account of intra- and inter- Molecular Bonding in Lanthanide Compounds – preprint DOI: 10.5281/zenodo.14225779; in progress of sending to *Computational Materials Science*

Book chapter

Fanica Cimpoesu, Maria-Cristina Buta, Ana Maria Toader and Gabriela Ionita. The Spin Chemistry of Nitroxide-Based Organic Biradicals: EPR Data and Computational Experiments. In *Fundamental and Biomedical Aspects of Redox Processes*, pp. 111-142. IGI Global, 2023.

Conference participations

Fănică Cimpoeșu, Ana Maria Toader, Maria Cristina Buta, Marilena Ferbințeanu
Particularities of Electronic Structure in Lanthanide Compounds. Modeling Optical Properties.

International Conference on Advanced Materials, Nanosciences and Applications & Training school in Spectroscopies for Environment and Nanochemistry (ICAMANA2022), november 22-24th 2022, Louvain-la-Neuve, Belgia, oral presentation

Fănică Cimpoeșu, Marilena Ferbințeanu, Werner Urland
Engineering Magnetic and Optical Properties of Lanthanide Compounds with Ligand Field Models

20th International Balkan Workshop on Applied Physics (IBWAP 2022), July 11-16th 2022, Constanța, România, oral presentation - invited

Ana Maria Toader, Maria Cristina Buta, Adela Mihai, Fănică Cimpoeșu
Assesing Computational Tools for Modeling Lanthanide-Based Luminscent Materials
20th International Balkan Workshop on Applied Physics (IBWAP 2022), July 11-16th 2022, Constanța, România, poster

Maria Cristina Buta, Ana Maria Toader, Corneliu I. Oprea, Mihai Gîrțu, Fănică Cimpoeșu
Mapping the Spin Coupling in Antioxidant Molecules
20th International Balkan Workshop on Applied Physics (IBWAP 2022), July 11-16th 2022, Constanța, România, poster

Fănică Cimpoeșu
Computational molecular magnetism and beyond. Exchange and spin-orbit coupling and other ingredients. *MolMod Lectures*, March 13th 2023, Cluj-Napoca, Romania, oral presentation, online

Fănică Cimpoeșu, Mihai Secu, Marilena Ferbințeanu
Structure-Property Correlations in the Chemistry and Spectroscopy of Lanthanide Compounds
21th International Balkan Workshop on Applied Physics (IBWAP 2023), July 11-14th 2023, Constanța, Romania, oral presentation - invited

Ana Maria Toader, Bogdan Frecus, Corneliu I. Oprea, Maria Cristina Buta
Assesing Quantum Calculation Methods for Ligand Field and Spectroscopy of Lanthanide Coordination Compounds
21th International Balkan Workshop on Applied Physics (IBWAP 2023), July 11-14th 2023, Constanța, Romania, poster

Maria Cristina Buta, Ana Maria Toader, Corneliu I. Oprea, Fănică Cimpoeșu
Modeling the Activity of Cytochrome P450-NO Reductase
21th International Balkan Workshop on Applied Physics (IBWAP 2023), July 11-14th 2023,
Constanța, Romania, poster

Fănică Cimpoeșu
A journey to the end of periodic table: the quantum chemistry of lanthanides.
Workshop on lanthanides systems, September 29th – October 1 2023, Muralto, Elvetia, oral
presentation - invited

Fănică Cimpoeșu
Understanding the mechanism of 4f-5d transitions of lanthanide ions inside of the fullerene
cages. *NanoMod 2023 - Research International Workshop – Third Edition*, October 21th
2023, Timisoara, oral presentation - invited, online

Fănică Cimpoeșu, Marilena Ferbinteanu
*Wave Function, Density Functional and Phenomenological Theories for Lanthanide Solid-
State Systems*
3rd International Conferences on Noncovalent Interactions (ICNI2024) – June 17-21th, 2024,
Belgrad, Serbia, oral presentation – invited

Fănică Cimpoeșu, Marilena Ferbinteanu
Lanthanide Ions in Crystals and Crystal Fields
3rd International Conferences on Noncovalent Interactions (ICNI2024) – June 17-21th, 2024,
Belgrad, Serbia, oral presentation – invited

Maria C. Buta, Ana M. Toader, Andreea-D. Zamfirescu, Corneliu I. Oprea, Fănică Cimpoeșu
Modeling Lanthanide Luminescence in Solid-State Fluorides
22th International Balkan Workshop on Applied Physics (IBWAP 2024), July 9-12th 2024,
Constanța, România, poster

Fănică Cimpoeșu, Marilena Ferbinteanu
Long-Range Effects in The Structure and Properties Of Lanthanide Compounds
22th International Balkan Workshop on Applied Physics (IBWAP 2024), July 9-12th 2024,
Constanța, România, oral presentation – invited

Ana M. Toader, B. Frecuș, I. Humelnicu, Maria C. Buta, Adela Mihai, Fănică Cimpoeșu
*The Confrontation of Wave Function and Density Functional Theories in The Field of
Lanthanide Compounds*
22th International Balkan Workshop on Applied Physics (IBWAP 2024), July 9-12th 2024,
Constanța, România, poster

Fănică Cimpoeșu, Marilena Ferbinteanu
*Experimental and theoretical structural chemistry in the frame of ligand field paradigms. An
old and evergreen field.*
Iași CHEM 2024 Conference, 6th Edition, October 31th – November 1 2024, Iași, Romania,
oral presentation - invited