

Results

Published articles

Ana Maria Toader, Bogdan Frecus, Corneliu I. Oprea, Maria Cristina Buta, Assessing Quantum Calculation Methods for the Account of Ligand Field in Lanthanide Compounds. *Physchem* 2023, 3, 270–289.

Alice Mischie, Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu, Harmonic oscillator model of aromaticity (HOMA) in conjugated radicals and cations. *Computational and Theoretical Chemistry*, 2023, 1230, 114370

Under review articles

Ana Maria Toader, Maria Cristina Buta, Werner Urland, Alessandro Stroppa, Fanica Cimpoesu, Assessing the lanthanide pseudopotential datasets in terms of Slater-Condon spectral parameters. *Computational Materials Science*, nr. manuscris COMMAT-D-23-02710

Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu, On the Calculation of Lanthanide Systems. The Spectral Parameters of Praseodymium Trivalent Ion. *Chemistry Journal of Moldova*. Ms. Ref no.: CJM-1146

Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu, Adela Mihai, The Holohedrization Effect in Ligand Field Models. *Symmetry*. Manuscript ID: symmetry-2785719.

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 Cimpoesu

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

Fănică Cimpoesu, 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 Cimpoescu
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 Cimpoescu

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

Fănică Cimpoescu

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