

Results 2017-2019

Articles (6)

M. Ferbințeanu, A. Stroppa, M. Scarrozza, I. Humelnicu, D. Maftai, B. Frecuș, F. Cimpoeșu

On The Density Functional Theory Treatment of Lanthanide Coordination Compounds: A Comparative Study in a Series of Cu–Ln (Ln = Gd, Tb, Lu) Binuclear Complexes

Inorganic Chemistry 2017, 56(16), pag. 9474–9485

Y. Gao, M. Viciano-Chumillas, A. M. Toader, S.J. Teat, M. Ferbințeanu, S. Tanase

Cyanide-bridged coordination polymers constructed from lanthanide ions and octacyanometallate building-blocks

Inorganic Chemistry Frontiers 5, 2018, 1967-1977

Ana M. Toader, Cristina M. Buta, Bogdan Frecus, Alice Mischie, Fanica Cimpoesu

Valence Bond Account of Triangular Polyaromatic Hydrocarbons with Spin: Combining Ab Initio and Phenomenological Approaches

J. Phys. Chem. C 2019, 123(11), 6869-6880

Ana M. Toader, Snezana D. Zaric , Christina M. Zalaru , Marilena Ferbinteanu.

The Structural Details of Aspirin Molecules and Crystals.

Current Medicinal Chemistry, 2019, 26, 1-22

Maria Cristina Buta, Ana Maria Toader, Bogdan Frecus, Corneliu I. Oprea, Fanica Cimpoesu and Gabriela Ionita

Molecular and Supramolecular Interactions in Systems with Nitroxide-Based Radicals

Int. J. Mol. Sci. 2019, 20(19), 4733

Ana M. Toader, Cristina M. Buta, Dan Maftai, Mihai V. Putz, Fanica Cimpoesu
Atoms in Generalized Orbital Configurations. Toward Atom-Dedicated Density Functionals.

Int. J. Mol. Sci. 2019, 20(23), 5943

Book chapter (2)

F. Cimpoesu, M. V. Putz, M. Ferbințeanu

Wave Function Theories and Electronic Structure Methods: Quantum Chemistry, from Atom to Molecules (Cap. 2), pp. 107-220, in

Structural Chemistry Principles, Methods, and Case Studies, Springer 2018

F. Cimpoesu, M. V. Putz, M. Ferbințeanu

Density Functional Theory: From Conceptual Level Toward Practical Functionality (Cap. 3), pp. 221-289, in

Structural Chemistry Principles, Methods, and Case Studies, Springer 2018

Conferences (19)

F. Cimpoesu

Revisiting the Methods of the Atomic Structure. Back to the Basis.

Iași Chem 2017, October 26-28, 2017, Iași, România, invited presentation.

Fanică Cimpoesu

Bond. Chemical Bond! Spying the Secrets of Molecular Structure with State-of-the-Art and Revisited Computation Methods.

Molecular modeling in chemistry and biochemistry MOLMOD 2018

Cluj-Napoca, 28-30 oct 2018, invited presentation

Alice Mischie, Ana Maria Toader, Fanică Cimpoesu

Hybrids and Bond Angles in Small Prototypic Hydrocarbon Molecules

Molecular modeling in chemistry and biochemistry MOLMOD 2018

Cluj-Napoca, 28-30 oct 2018, poster

Ana-Maria Toader, Fanică Cimpoeșu

Reshaping the Principles and Techniques of Gaussian-type Basis Sets in Computational Chemistry

Molecular modeling in chemistry and biochemistry MOLMOD 2018

Cluj-Napoca, 28-30 oct 2018, poster.

Cristina Maria Buta, Ana Maria Toader, Gabriela Ioniță

Through-space and Trough-solvent Interactions between Nitroxide-based Stable Radicals.

Molecular modeling in chemistry and biochemistry MOLMOD 2018

Cluj-Napoca, 28-30 oct 2018, poster.

Fănică Cimpoeșu, Marilena Ferbințeanu

Structure-properties rationales for the use of rich data from optical spectra and magnetism of lanthanides

4th International Conference on Analytical Chemistry ROICAC 2018, București, 1-3 sept 2018, invited presentation.

Maria-Cristina Buta, Ana Maria Toader, Fănică Cimpoeșu

Modeling the long-range coupling in spin-probe systems

4th International Conference on Analytical Chemistry ROICAC 2018, București, 1-3 sept 2018, poster

Fănică Cimpoeșu

Revisiting key elements of computational chemistry

43rd International Conference on Coordination Chemistry, ICC2018, Sendai, Japonia, 30 iulie 4 august 2018, presentation.

A.M. Toader, C. M. Buta, A. Mischie, N. Spătaru, C. Oprea, F. Cimpoeșu

Charge Transfer Processes Modeled Within Spin Coupling And Vibronic Paradigms

18th International Balkan Workshop on Applied Physics IBWAP 2018,
Constanta, 9-13 iulie 2018, poster

C. M. Buta, A. M. Toader, C. Oprea, G. Ioniță, F. Cimpoesu

Magneto-Structural Correlations with Nitroxide Radicals

18th International Balkan Workshop on Applied Physics IBWAP 2018,
Constanta, 9-13 iulie 2018, poster.

Ana Maria Toader, Fania Cimpoesu

Reforming elements of computational chemistry.

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD
2018, Timisoara, 15-18 mai 2018, invited presentation.

Ana Maria Toader, Cristina Maria Buta, Fănică Cimpoesu

*On the Electronic Structure of Triangular Polyaromatic Hydrocarbons with
Spin*

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD
2018, Timisoara, 15-18 mai 2018, poster

Maria Cristina Buta, Ana Maria Toader, Gabriela Ioniță

Structural analyses of interacting nitroxide-based organic radicals.

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD
2018, Timisoara, 15-18 mai 2018, poster

Alice Mischie, Ana Maria Toader, Fania Cimpoesu

Revisiting ring strain with combined quantum techniques.

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD
2018, Timisoara, 15-18 mai 2018, poster.

Marilena Ferbinteanu, Fănică Cimpoesu

Electronic Structure Particularities of Lanthanide Ions in Molecules

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD 2019, Timisoara, 22-23 aprilie 2019, invited presentation

Ana Maria Toader, Stefania Tanase, Marilena Ferbinteanu, Fănică Cimpoescu

Modeling of Cyanide-Bridged Lanthanide-based Coordination Polimers

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD 2019, Timisoara, 22-23 aprilie 2019, poster

Cristina Maria Buta, Alice Mischie, Gabriela Ionita, Marilena Ferbinteanu

The Modeling of Square-Pyramidal Mixed Ligand Copper Complexes

Nano-Modeling of Strategic Materials for Knowledge Economy NANO-MOD 2019, Timisoara, 22-23 aprilie 2019, poster

A.M. Toader, C. M. Buta, B. Frecus, A. Mischie, F. Cimpoescu

Triangular Polyaromatic Hydrocarbons with Spin

19th International Balkan Workshop on Applied Physics IBWAP 2019, Constanta, 16 - 19 iulie 2019, poster

C. I. Oprea, A. M. Toader, F. Cimpoescu, A. Ndiaye, M. Gîrțu

First Principle Studies of Charge Transfer in Model Systems Representative for Dye-Sensitized Solar Cells

19th International Balkan Workshop on Applied Physics IBWAP 2019, Constanta, 16 - 19 iulie 2019, poster