

## Rezultate 2017-2019

### Articole (6)

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

*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* 56(16), 2017, 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), pag. 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

### **Capitol carte (2)**

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

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

*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), pag. 221-289, în

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

### **Conferințe (19)**

F. Cimpoesu

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

Iași Chem 2017, 26-28 Octombrie 2017, Iași, România, prezentare orală, invitat

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, prezentare orală, invitat

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 Cimpoescu

*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 Cimpoescu, 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, prezentare orală, invitat

Maria-Cristina Buta, Ana Maria Toader, Fănică Cimpoescu

*Modeling the long-range coupling in spin-probe systems*

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

Fănică Cimpoescu

*Revisiting key elements of computational chemistry*

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

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

*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 Corelations with Nitroxide Radicals*

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

Ana Maria Toader, Fanica Cimpoesu

*Reforming elements of computational chemistry.*

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

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, Fanica 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, prezentare orală, invitat

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