

## Results

7 ISI papers were contracted and 14 ISI papers were realized.

In addition we produced

4 chapters book (Springer and IGI Global publishers)

1 book (Springer publishers),

*All papers, book chapters and the book acknowledged the UEFISCDI support.*

24 conferences (invited lectures, keynotes, oral presentations, posters, in national and international events) are published.

### Articole/Papers (14)

Toader, A.M.; Buta, C.; Frecus, B.; Diudea, M.; Cimpoesu, F.

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

*J. Chem. Theory Comput.* **2016**, submitted.

Cimpoesu, F.; Buta, C.; Ferbinteanu, M.; Philpott, M.R.; Stroppa, A.; Putz, M.

*Electronic Structure of Linear Polyacenes*

*Curr. Org. Chem.*, **2016**, in press.

Frecus, B.; Buta, C.M.; Oprea, C.I.; Stroppa, A.; Putz, M.V.; Cimpoesu, F.

*Noble gas endohedral fullerenes, Ng@C-60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations*  
*Theor. Chem. Acc.* **2016**, 135(5), 133 (1-9), DOI: 10.1007/s00214-016-1883-z (IF:1.806)

Oprea, C.; Petcu, L.C.; Girtu, M.

*DFT Study of Binding and Electron Transfer from Penicillin to a TiO<sub>2</sub> Nanocluster: Applications to Photocatalytic Degradation*

*E-Health and Bioengineering - EHB 2015*, DOI: 10.1109/EHB.2015.7391481,

Ramanantoanina, H.; Urland, W.; Herden, B.; Cimpoesu, F.; Daul, C.

*Tailoring the optical properties of lanthanide phosphors: prediction and characterization of the luminescence of Pr(3+)-doped LiYF<sub>4</sub>.*

*Phys. Chem. Chem. Phys. PCCP*, **2015**, 17(14), 9116-9125. (IF:4.19)

Ramanantoanina, H.; Sahnoun, M.; Barbiero, A.; Ferbinteanu, M.; Cimpoesu, F.

*Development and applications of the LFDFT: the non-empirical account of ligand field and the simulation of the f-d transitions by density functional theory*

*Phys. Chem. Chem. Phys.* **2015**, 17(28), 18547-18557.

DOI: 10.1039/c5cp02349a, WOS:000357808500037. (IF:4.493).

Garcia-Fuente, A.; Cimpoesu, F.; Ramanantoanina, H.; Herden, B.; Daul, C.; Suta, M.; Wickleder, C.; Urland, W.

*A ligand field theory-based methodology for the characterization of the Eu<sup>2+</sup> [Xe]4f(6)5d(1) excited states in solid state compounds*

*Chem. Phys. Lett.* **2015**, 622, 120-123. DOI: 10.1016/j.cplett.2015.01.031. (IF:1.991)

Ramanantoanina, H.; Cimpoesu, F.; Gottel, C.; Sahnoun, M.; Herden, B.; Suta, M.; Wickleder, C.; Urland, W.; Daul, C.  
*Prospecting Lighting Applications with Ligand Field Tools and Density Functional Theory: A First-Principles Account of the 4f7-4f65d1 Luminescence of CsMgBr3:Eu2+*  
*Inorg. Chem.* **2015**, 54(17), 8319-8326, DOI: 10.1021/acs.inorgchem.5b00988. (IF: 4.82)

Cimpoesu, F.; Frecus, B.; Oprea, C.I.; Ramanantoanina, H.; Urland, W.; Daul, C.  
*On exchange coupling and bonding in the Gd2@C80 and Gd2@C79N endohedral dimetallo-fullerenes,*  
*Mol. Phys.* **2015**, 113(13-14), 1712-1727, DOI:10.1080/00268976.2015.1007107 (IF:1.642)

Ramanantoanina, H.; Urland, W.; García-Fuente, A.; Cimpoesu, F.; Daul, C.  
*Ligand field density functional theory for the prediction of future domestic lighting*  
*Phys. Chem. Chem. Phys.* **2014**, 16(28), 14625-14634. Advance Article (DOI: 10.1039/C3CP55521F). (IF:4.19)

Frecus, B.; Oprea, C.I.; Panait, P.; Ferbinteanu, M.; Cimpoesu, F.; Gîrțu, M. A.  
*Ab initio study of exchange coupling for the consistent understanding of the magnetic ordering at room temperature in V[TCNE] (x)*  
*Theor. Chem. Acc.* **2014**, 133,1470. (DOI: 10.1007/s00214-014-1470-0) (IF:2.143)

Cimpoesu, F.; Frecus, B.; Oprea, C.I.; Panait, P., Gîrțu, M. A.  
*Disorder, exchange and magnetic anisotropy in the room-temperature molecular magnet V[TCNE](x) - A theoretical study,*  
*Comp. Mat. Sci.* **2014**, 91, 320-328. (DOI: 10.1016/j.commatsci.2014.04.062) (IF:1.879)

Ramanantoanina, H.; Urland, W.; Cimpoesu, F.; Daul, C.  
*The angular overlap model extended for two-open-shell f and d electrons,*  
*Phys. Chem. Chem. Phys.* **2014**, 16, 12282-12290. (DOI: 10.1039/C4CP01193G). (IF:4.19)

Cimpoesu, F.; Dragoie, N.; Ramanantoanina, H.; Urland, W.; Daul, C.  
*The theoretical account of the ligand field bonding regime and magnetic anisotropy in the DySc2N@C80 single ion magnet endohedral fullerene,*  
*Phys. Chem. Chem. Phys.* **2014**, 16, 11337-11348.(DOI: 10.1039/C4CP00953C). (IF:4.19)

#### Capitole de carte/ Chapters book (4)

Putz, M.V.; Cimpoesu, F.; Ferbinteanu, M.  
*New keys for Old Keywords. Hybridization and Aromaticity, Graphs and Topology*  
*In Structural Chemistry Principles, Methods, and Case Studies, Springer, 2017, in press.*

Ferbinteanu, M.; Buta, C.; Toader, A.M.; Cimpoesu, F.  
*The Spin Coupling in the Polyaromatic Hydrocarbons and Carbon-based Materials*  
*In Organic synthesis and carbon related materials- Dedicated to Nobel Laureate Prof. Akira Suzuki for his 85th birthday, Springer, 2017, in press.*

Ferbinteanu, M.; Ramanantoanina, H.; Barbiero, A.; Cimpoesu, F.  
*Bonding mechanisms and causal relationships with magnetic properties in extended coordination systems: Case studies in the challenge of property design at nanoscale*, IGI publisher, Volume Title: *Sustainable Nanosystems Development, Properties, And Applications*, Volume Editors: Mihai V. Putz & Marius C. Mirica, 2017, in press. ISBN13: 9781522504924 DOI: 10.4018/978-1-5225-0492-4

Ferbinteanu, M.; Cimpoesu, F.; Tanase, S.  
*Metal-Organic Frameworks with d-f Cyanide Bridges: Structural Diversity, Bonding Regime, and Magnetism*,  
in *Lanthanide Metalorganic Frameworks*, Ed. Peng Cheng,  
*Structure and Bonding* **2015**, 163, 185-229,  
ISBN: 978-3-662-45772-6 (Print) 978-3-662-45773-3 (Online)  
DOI: 10.1007/430\_2014\_156M, WOS:000348907100007

### **Carti/Books (1)**

Putz, M.V.; Cimpoesu, F.; Ferbinteanu, M. *Structural Chemistry Principles, Methods, and Case Studies*, Springer, **2017**, 800 pag., in press

### **Conferinte / Conferences (24)**

M. Ferbinteanu, F. Cimpoesu, *The Magnetic Anisotropy, from Complex Units to Nano-Scale Level*, 2013 JSAP-MRS Joint Symposium, Kyoto, Japan, September, 16-20, 2013, invited presentation.

F. Cimpoesu, *New keys for old keywords: Ligand Field theory, revisited*. International Conference of Physical Chemistry ROMPHYSICHEM15, Bucharest, Romania, September 9-13, 2013, keynote presentation.

D. Humelnicu, I. Humelnicu, P. Badica, M. Ferbinteanu, *Complexes of Keggin-type monolacunary heteropolytungstates with lanthanides: synthesis and magnetic properties*, International Conference of Physical Chemistry ROMPHYSICHEM15, Bucharest, Romania, September 9-13, 2013, poster.

F. Cimpoesu, *Assessing the ab initio methods to account Ligand Field in Lanthanide complexes*, International Conference on Molecular Magnetism, Jujols VII, January 13-17, 2014, Muellheim, Germany, oral presentation

F. Cimpoesu, *Property Engineering with Modeling and Computational tools. Charge Transfer and Electronic Transitions in Complex Units*, The 14th International Balkan Workshop on Applied Physics and Materials Science, Constanta, Romania, July 2-4, 2014, oral presentation.

F. Cimpoesu, *Prospecting the properties of lanthanide-based systems with new modeling*, Advances workshop in solar energy conversion and nanophysics, Bucharest, Romania, September 2014, oral presentation.

F. Cimpoesu, *Back to the Basis! Revisiting Some Methodological Issues of Computational Chemistry*, Molecular Modelling in Chemistry and Biochemistry, MOLMOD2014, Cluj-Napoca, Romania, November 13-15, 2014, invited lecture.

F. Cimpoesu, *New insights in the bonding regime and ligand field in coordination complexes. A density functional study*, Summer School on Applied Supramolecular Chemistry and Workshop on Theoretical Supramolecular Chemistry, July 28-30, 2014, invited lecture.

F. Cimpoesu, M. Ferbinteanu, *The Vibrational Chemistry of the Spin-Crossover Phenomena. New Case Studies.*, 15th International Balkan Workshop on Applied Physics, 2-4 July 2015 Constanta, ROMANIA, invited lecture.

M. Ferbinteanu, F. Cimpoesu, *Bonding Mechanisms And Causal Relationships with Magnetic Properties in Extended Coordination Systems. Case Studies in the Challenge of Property Design at Nanoscale.*, The 8th International Conference On Advanced Materials: ROCAM 2015, 7-10 July 2015, Bucharest, Romania, oral presentation. Abstract Book, editura Granada, ISSN 1842-3574., p.158

A. Stroppa, D. Di Sante, P. Barone, M. Bokdam, G. Kresse, C. Franchini, M.-H. Whangbo, I. Humelnicu, S. Picozzi, *Tunable Ferroelectric Polarization and Its Interplay with Spin-Orbit Coupling in Perovskite Halide Solar Cells*, The 8th International Conference On Advanced Materials: ROCAM 2015, July 7-10, 2015, Bucharest, Romania, oral presentation.

M. Ferbinteanu, F. Cimpoesu, *Discovering the Poles of the Molecular Magnets*, The 2nd International Conference on Advanced Complex Inorganic Nanomaterials, ACIN 2015, 13th-17th July 2015, Namur, Belgium, oral presentation.

M. Ferbinteanu, F. Cimpoesu, *Molecular Assembling and Magnetic Manifestations in 2D Systems and Related Edifices. Structure-property Relationships in Case Studies.*, The 76th Japanese Society of Applied Physics Autumn Meeting, JSAP2015, 13th-16th September 2015, Nagoya, Japan, invited lecture.

F. Cimpoesu, *Spin Coupling in Carbon Based Materials*, Nanoscience in Chemistry, Physics, Biology And Mathematics, 12-14 Nov. 2015, Cluj, Romania, invited lecture.

M. Ferbinteanu, F. Cimpoesu, *Mapping the Single Molecule Magnet Behaviour in f-Type Complexes*, 16th International Balkan Workshop on Applied Physics, Proceeding IBWAP Constanta, Romania, July 7-9, 2016, invited lecture.

M.C. Buta, F. Cimpoesu, *Frequency Shifts in Vibration Spectra of Ng@C60 versus C60 systems (Ng=Ar, Kr)*, CM1305 ECOSTBio Summer School Groningen (Theory and Practice in Spectroscopy and Electrochemistry), Groningen, Netherlands, July 9-16, 2016, poster.

M. Ferbinteanu, F. Cimpoesu, *Mapping the Ligand Field and Magnetic Anisotropy in f-type Complexes.*, The 15th International Conference on Molecule-Based Magnets-Book of abstracts, ICMM2016, Sendai, Japan, September 4-8, 2016, oral and poster presentation.

W. Urland, F. Cimpoesu, *A new generation of problems in the ligand field modelling. From phenomenology to first principles prediction of optical properties*, 16th International Conference of Physical Chemistry ROMPHYSICHEM-16, Galati, Romania, September 21-23, 2016, oral presentation.

M. Ferbinteanu, F. Cimpoesu, *New keys for the keywords of molecular magnetism. A chemist's perspective on the magnetic anisotropy*, 16th International Conference of Physical Chemistry ROMPHYSICHEM-16, Galati, Romania, September 21-23, 2016, oral presentation.

I. Humelnicu, D. Maftai, B. Frecus, F. Cimpoesu, A. Stroppa, *On the density functional theory treatment of lanthanide coordination compounds. Challenging the limits with relevant computational experiments*, 16th International Conference of Physical Chemistry ROMPHYSICHEM-16, Galati, Romania, September 21-23, 2016, poster.

A. Toader, T. Spataru, N. Spataru, F. Cimpoesu, *Electron Structure Effects in Boron Doped Diamond*, 16th International Conference of Physical Chemistry ROMPHYSICHEM-16, Galati, Romania, September 21-23, 2016, poster.

C. I. Oprea, F. Cimpoesu, W. Urland, *On exchange coupling and bonding in the Gd<sub>2</sub>@C<sub>80</sub> and Gd<sub>2</sub>@C<sub>79N</sub> endohedral dimetallo-fullerenes*, 16th International Conference of Physical Chemistry ROMPHYSICHEM-16, Galati, Romania, September 21-23, 2016, poster.

M.C. Buta, M. Turcu, M. Iote, M. Radu, M. Ferbinteanu, F. Dumitrascu, C. Draghici, R. Tatia, L. Moldovan, I. Ardelean, Ch. Zalaru, *Novel aminopyrazole derivatives biologically active. Structural analysis.*, 16th International Conference of Physical Chemistry ROMPHYSICHEM-16, Galati, Romania, September 21-23, 2016, poster.

F. Cimpoesu, *A New Generation of Problems in the Ligand Field Modelling. From Phenomenology to First Principles Prediction of Optical Properties.*, Molecular modeling in chemistry and biochemistry MOLMOD 2016, Cluj-Napoca, Romania, November 13-15, 2016, invited lecture.