

Titlu proiect: Dezvoltari metodologice si experimente teoretice asupra regimului de legatura si proiectarea proprietatilor. De la atomi, la supra-molecule.

Categoria de proiect: IDEI, Proiect de cercetare exploratorie

Contractul de finanțare: Nr. 14/2013

Manager proiect: Dr. Fanica Cimpoesu

Lista rezultate

Nr. crt.	NUME AUTORI	TITLUL ARTICOLULUI/ CĂRȚII / COMUNICĂRII ȘTIINȚIFICE	REVISTA / VOLUMUL/EDITURA IN CARE A APARUT / CONFERINTA LA CARE S-A COMUNICAT	ANUL PUBLICĂRII/ COMUNICĂRII
ARTICOLE ISI				
1	Cimpoesu Fanica, Dragoe Nita, Ramanantoanina Harry, Urland Werner, Daul Claude A.	The Theoretical Account of the Ligand Field Bonding Regime and Magnetic Anisotropy in the DySc2N@C80 Single Ion Magnet Endohedral Fullerene.	PHYSICAL CHEMISTRY CHEMICAL PHYSICS/ Vol. 16	2014
2	Ramanantoanina Harry, Urland Urland, Cimpoesu Fanica, Daul Claude	The Angular Overlap Model extended for two- open-shell f and d electrons	PHYSICAL CHEMISTRY CHEMICAL PHYSICS/ Vol. 16	2014
3	Ramanantoanina Harry, Urland Werner, Garcia- Fuente Amador, Cimpoesu Fanica, Daul Claude	Ligand field density functional theory for the prediction of future domestic lighting	PHYSICAL CHEMISTRY CHEMICAL PHYSICS/ Vol. 16	2014
4	Cimpoesu Fanica, Frecus Bogdan, Oprea Corneliu, Panait Petre, Girtu Mihai	Disorder, exchange and magnetic anisotropy in the room-temperature molecular magnet V[TCNE](x) - A theoretical study	COMPUTATIONAL MATERIALS SCIENCE/ Vol. 91	2014
5	Frecus Bogdan,	Ab initio study of	THEORETICAL	2014

	Oprea Corneliu, Panait Petre, Ferbinteanu Marilena, Cimpoesu Fanica, Girtu Mihai	exchange coupling for the consistent understanding of the magnetic ordering at room temperature in V[TCNE] (x)	CHEMISTRY ACCOUNTS/ Vol. 133	
6	Cimpoesu Fanica, Frecus Bogdan, Oprea Corneliu, Ramanantoanina Harry, Urland Werner, Daul Claude	On Exchange Coupling and Bonding in the Gd ₂ @C ₈₀ and Gd ₂ @C ₇₉ N Endohedral Dimetallo-Fullerenes	MOLECULAR PHYSICS/ Vol. 113	2015
7	Cimpoesu Fanica, Ramanantoanina Harry, Goettel Christian, Sahnoun Mohammed, Herden Benjamin, Suta Markus, Wickleder Claudia, Urland Werner, Daul Claude	Prospecting Lighting Applications with Ligand Field Tools and Density Functional Theory: A First-Principles Account of the 4f(7)-4f(6)5d(1) Luminescence of CsMgBr ₃ :Eu ²⁺	INORGANIC CHEMISTRY/ Vol. 54	2015
8	Cimpoesu Fanica, Garcia- Fuente Amador, Ramanantoanina Harry, Herden Benjamin, Daul Claude, Suta Markus, Wickleder Claudia, Urland Werner	A ligand field theory-based methodology for the characterization of the Eu ²⁺ [Xe]4f(6)5d(1) excited states in solid state compounds	CHEMICAL PHYSICS LETTERS/ Vol. 622	2015
9	Cimpoesu Fanica, Ramanantoanina Harry, Sahnoun Mohammed, Barbiero Andrea, Ferbinteanu Marilena	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	PHYSICAL CHEMISTRY CHEMICAL PHYSICS/ Vol. 17	2015

10	Cimpoesu Fanica, Ramanantoanina Harry, Urland Werner, Herden Benjamin, Daul Claude	Tailoring the optical properties of lanthanide phosphors: prediction and characterization of the luminescence of Pr ³⁺ -doped LiYF ₄	PHYSICAL CHEMISTRY CHEMICAL PHYSICS/ Vol. 17	2015
11	Cimpoesu Fanica, Oprea Corneliu, Buta Cristina, Frecus Bogdan, Stroppa Alessandro, Putz Mihai	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	THEORETICAL CHEMISTRY ACCOUNTS/ Vol. 135	2016
12	Cimpoesu Fanica, Buta Cristina, Ferbinteanu Marilena, Philpott Michael R., Stroppa Alessandro, Putz Mihai	Electronic Structure of Linear Polyacenes	CURRENT ORGANIC CHEMISTRY/ Vol. 21	2017
	ARTICOLE ALTE BAZE DE DATE			
1	Oprea Corneliu, Lucian C., Girtu Mihai	DFT Study of Binding and Electron Transfer from Penicillin to a TiO ₂ Nanocluster: Applications to Photocatalytic Degradation	The 5th IEEE International Conference on E-Health and Bioengineering - EHB 2015	2015

CARTI				
1	Ferbinteanu Marilena, Cimpoesu Fanica, Tanase Stefania	Metal-Organic Frameworks with d-f Cyanide Bridges: Structural Diversity, Bonding Regime, and Magnetism Capitol in LANTHANIDE METAL- ORGANIC FRAMEWORKS Book Series: Structure and Bonding	SPRINGER-VERLAG Springer Berlin Heidelberg BERLIN, HEIDELBERGER PLATZ 3, D-14197 BERLIN, GERMANY	2015
2	Cimpoesu Fanica, Ramanantoanina Harry, Ferbinteanu Marilena	Case Studies in the Challenge of Properties Design at Nanoscale: Bonding Mechanisms and causal Relationship – Capitol in Sustainable Nanosystems Development, Properties, and Applications	IGI Global	2016
3	Cimpoesu Fanica, Buta Cristina, Ferbinteanu Marilena, Toader Ana Maria	The Spin Coupling in the Polyaromatic Hydrocarbons and Carbon-based Materials – Capitol in Organic synthesis and carbon related materials: Polymers, carbon nanocomposites, graphene - Dedicated to Nobel Laureate Prof. Akira Suzuki for his 85th birthday	SPRINGER-VERLAG Springer Berlin Heidelberg BERLIN, HEIDELBERGER PLATZ 3, D-14197 BERLIN, GERMANY	2017

COMUNICARI STIINTIFICE NATIONALE				
1	Cimpoesu Fanica	New keys for old keywords: Ligand Field theory	ROMPHYSICHEM15, 11-13/09/2013, Bucuresti	2013
2	Humelnicu Doina, Humelnicu Ionel, Badica Petre, Ferbinteanu Marilena	Complexes of Keggin-type monolacunary heteropolytungstates with lanthanides: synthesis and magnetic properties	ROMPHYSICHEM15, 11-13/09/2013, Bucuresti	2013
3	Cimpoesu Fanica	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, 02-04/07/2014, Constanta	2014
4	Cimpoesu Fanica	Prospecting the properties of lanthanide-based systems with new modelling methodologies	Advances workshop in solar energy conversion and nanophysics, 01-03/09/2014, Magurele	2014
5	Cimpoesu Fanica	Back to the Basis! Revisiting Some Methodological Issues of Computational Chemistry	MOLMOD2014, 13-15/11/2014, Cluj-Napoca	2014
6	Cimpoesu Fanica, Ferbinteanu Marilena	The Vibrational Chemistry of the Spin-Crossover Phenomena. New Case Studies	IBWAP 2015, 02-04/07/2015, Constanta	2015
7	Cimpoesu Fanica, Ferbinteanu Marilena	Bonding Mechanisms And Causal Relationships with Magnetic Properties in Extended Coordination Systems. Case Studies in the Challenge of Property Design at	The 8th International Conference On Advanced Materials: ROCAM 2015, 07-10/07/2015, Bucuresti	2015

		Nanoscale.		
8	Humelnicu Ionel, Stroppa Alessandro	Tunable Ferroelectric Polarization and Its Interplay with Spin- Orbit Coupling in Perovskite Halide Solar Cells	The 8th International Conference On Advanced Materials: ROCAM 2015, 07-10/07/2015, Bucuresti	2015
9	Cimpoesu Fanica	Spin Coupling in Carbon Based Materials	Nanoscience in Chemistry, Physics, Biology And Mathematics, 12-14/11/2015, Cluj-Napoca	2015
10	Ferbinteanu Marilena, Cimpoesu Fanica	Mapping the Single Molecule Magnet Behaviour in f-Type Complexes	International Balkan Workshop on Applied Physics IBWAP, 07- 09/07/2016, Constanta	2016
11	Cimpoesu Fanica, Urand Werner	A new generation of problems in the ligand field modelling. From phenomenology to first principles prediction of optical properties	ROMPHYSICHEM15, 21-24/09/2016, Galati	2016
12	Cimpoesu Fanica, Ferbinteanu Marilena	New keys for the keywords of molecular magnetism. A chemist's perspective on the magnetic anisotropy	ROMPHYSICHEM15, 21-24/09/2016, Galati	2016
13	Cimpoesu Fanica, Oprea Corneliu, Urand Werner	On exchange coupling and bonding in the Gd ₂ @C ₈₀ and Gd ₂ @C ₇₉ N endohedral dimetallo-fullerenes	ROMPHYSICHEM15, 21-24/09/2016, Galati	2016
14	Cimpoesu Fanica, Humelnicu Ionel, Maftai Dan, Frecus Bogdan, Stroppa Alessandro	On the density functional theory treatment of lanthanide coordination compounds. Challenging the limits with relevant computational experiments	ROMPHYSICHEM15, 21-24/09/2016, Galati	2016

15	Cimpoesu Fanica, Toader Ana Maria, Spataru Tanta, Spataru Nicolae	Electron Structure Effects in Boron Doped Diamond	ROMPHYSICHEM15, 21-24/09/2016, Galati	2016
16	Buta Cristina	Novel aminopyrazole derivatives biologically active. Structural analysis	ROMPHYSICHEM15, 21-24/09/2016, Galati	2016
17	Cimpoesu Fanica	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, 13-15/11/2016, Cluj-Napoca	2016
COMUNICARI STIINTIFICE INTERNATIONALE				
1	Cimpoesu Fanica, Ferbinteanu Marilena	The Magnetic Anisotropy, from Complex Units to Nano-Scale Level	2013 JSAP-MRS Joint Symposium, 16-20/09/2013, Kyoto, Japonia	2013
2	Cimpoesu Fanica	Assessing the ab initio methods to account Ligand Field in Lanthanide complexes	International Conference on Molecular Magnetism, Jujols VII, 13-17/01/2014, Mülheim a.d. Ruhr, Germania	2014
3	Cimpoesu Fanica	New insights in the bonding regime and ligand field in coordination complexes. A density functional study.	SUPRACHEM2014, 28- 01/08/2014, Belgrad, Serbia	2014
4	Cimpoesu Fanica, Ferbinteanu Marilena	Discovering the Poles of the Molecular Magnets	The 2nd International Conference on Advanced Complex Inorganic Nanomaterials, ACIN 2015, 13-17/07/2015, Namur, Belgia	2015
5	Cimpoesu Fanica, Ferbinteanu Marilena	Molecular Assembling and MMagnetic Manifestations in 2D Systems and Related Edifices. Structure- property	The 76th Japanese Society of Applied Physics Autumn Meeting, JSAP2015, 13- 16/09/2015, Nagoya, Japan	2015

		Relationships in Case Studies		
6	Buta Cristina, Cimpoesu Fanica	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), 09-16/07/2016, Groningen, Olanda	2016
7	Cimpoesu Fanica, Ferbinteanu Marilena	Mapping the Ligand Field and Magnetic Anisotropy in f-type Complexes.	The International Conference on Molecule-Based Magnets ICMM, 04-08/09/2016, Sendai, Japonia	2016
ATLASE, DICTIONARE DE SPECIALITATE				
1				
n				
CERERI BREVET DE INVENTII/BREVET OBTINUT				
1				
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ALTE rezultate				
1				
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Lista achizițiilor realizate în cadrul proiectului

Denumire echipament	Categorie de achiziții*: (numai mijloace fixe)	Valoarea (lei)	Locație
Computer portabil tip II	Calculatoare si accesorii	4.960,00	Institutul de Chimie-Fizica I. Murgulescu
Computer portabil tip I	Calculatoare si accesorii	2.480,00	Institutul de Chimie-Fizica I. Murgulescu
Imprimanta laser HP A4 Pro P1102	Calculatoare si accesorii	524,69	Institutul de Chimie-Fizica I. Murgulescu
Sursa ATX 450W	Calculatoare si accesorii	161,20	Institutul de Chimie-Fizica I. Murgulescu
HDD extern Seagate 500GB	Calculatoare si accesorii	690,06	Institutul de Chimie-Fizica I. Murgulescu
Computer de mare putere tip server	Calculatoare si accesorii	62.320,41	Institutul de Chimie-Fizica I. Murgulescu

Licenta soft stiintific Cambridge Structural Database	Program calculator	4.528,38	Institutul de Chimie-Fizica I. Murgulescu
Computer de mare putere tip server-plata partiala	Calculatoare si accesorii	30.000,00	Institutul de Chimie-Fizica I. Murgulescu
UPS cu adisare si control tensiune alimentare/iesire, frecventa, putere aparenta/reala	Calculatoare si accesorii	6.501,47	Institutul de Chimie-Fizica I. Murgulescu
Videoproiector Benq MX525	Calculatoare si accesorii	2.099,99	Institutul de Chimie-Fizica I. Murgulescu
Laptop lenovo idea pad intel dual core 1.1GHz, 8GB	Calculatoare si accesorii	6.908,98	Institutul de Chimie-Fizica I. Murgulescu
HDD extern portabil 1TB c husa	Calculatoare si accesorii	349,80	Institutul de Chimie-Fizica I. Murgulescu
Imprimanta multifunctionala HPDeskjet 4515	Calculatoare si accesorii	449,90	Institutul de Chimie-Fizica I. Murgulescu
Sistem de calcul exoria 6500-3 buc, laptop dell Inspiron 5558-1 buc	Calculatoare si accesorii	30.380,00	Institutul de Chimie-Fizica I. Murgulescu
Configuratii informatice Workstation Intel Core i7-6700K (4 cores, 8MB cache, 4GHz, 32 GB, SSD 240GB, HDD 3TB, Windows, mouse, keyboard	Calculatoare si accesorii	18.930,00	Institutul de Chimie-Fizica I. Murgulescu
Configuratii informatice Laptop Intel Core i7-6500U 2.5GHz, 15.6', 8GB, 1Tb, DVD-	Calculatoare si accesorii	5.220,00	Institutul de Chimie-Fizica I. Murgulescu

RW, AMD 2GB, Windows			
Configuratii informatic Laptop Intel Core i7-7500U 2.7GHz, 14', 8GB, 256GBSSD, Windows	Calculatoare si accesorii	5.556,00	Institutul de Chimie-Fizica I. Murgulescu
Pachete software matematice sau previzionale	Program calculator	12.960,00	Institutul de Chimie-Fizica I. Murgulescu
Configuratii electronice Licenta software Cloud Office 365 Home premium 5 utilizatori	Program calculator	978,00	Institutul de Chimie-Fizica I. Murgulescu

**Director proiect,
Dr. Fanica Cimpoesu**