

## LISTA PUBLICAȚIILOR

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WoS Researcher-ID: <https://www.webofscience.com/wos/author/record/C-4655-2012>

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### Teza de doctorat

„Density Functional Response Theory with Applications to Electron and Nuclear Magnetic Resonance”, C. I. Oprea, Theoretical Chemistry, School of Biotechnology, Royal Institute of Technology, Stockholm 2007, ISBN 978-91-7178-675-3

### Articole publicate în jurnale ISI:

1. „A Combined Experimental and Computational Study of Chrysanthemine as a Pigment for Dye-Sensitized Solar Cells”, A. Ndiaye, A. Dioum, C. I. Oprea, A. Dumbravă, J. Lungu, A. Georgescu, F. Moscalu, M. A. Gîrțu, A. C. Beye, I. Youm, *Molecules* **26**, 225, 1-15 (2021)
2. „Photoexcitation Processes in Oligomethine Cyanine Dyes for Dye-Sensitized Solar Cells—Synthesis and Computational Study”, C. I. Oprea, P. Panait, Z. M. Essam, R. M. Abd El-Aal, M. A. Gîrțu, *Nanomaterials* **10**, 662, 1-25 (2020)
3. “Molecular and Supramolecular Interactions in Systems with Nitroxide-based Radicals”, M. C. Buta, A. M. Toader, B. Frecus, C. I. Oprea, F. Cimpoesu, G. Ionita, *International Journal of Molecular Sciences* **20** (19), 4733, 1-20 (2019)
4. „Structure and Electronic Properties of TiO<sub>2</sub> Nanoclusters and Dye–Nanocluster Systems Appropriate to Model Hybrid Photovoltaic or Photocatalytic Applications”, C. I. Oprea, M. A. Gîrțu, *Nanomaterials* **9**, 357, 1-31 (2019)
5. “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”, B. Frecus, C. M. Buta, C. I. Oprea, A. Stroppa, M. V. Putz, F. Cimpoesu, *Theoretical Chemistry Accounts* **135** (5), 133, 1-9 (2016)
6. “On exchange coupling and bonding in the Gd<sub>2</sub>@C<sub>80</sub> and Gd<sub>2</sub>@C<sub>79</sub>N endohedral dimetallo-fullerenes”, F. Cimpoesu, B. Frecus, C. I. Oprea, H. Ramanantoanina, W. Urland, C. Daul, *Molecular Physics* **113**, 1712-1727 (2015)
7. „DFT Study of Binding and Electron Transfer from Colorless Aromatic Pollutants to a TiO<sub>2</sub> Nanocluster—Applications to Photocatalytic Degradation under Visible Light Irradiation”, C. I. Oprea, P. Panait, M. A. Gîrțu, *Beilstein Journal of Nanotechnology* **5**, 1016-1030 (2014)
8. „Elementary tight-binding method for simple electronic structure calculations - An educational approach to modeling conjugated dyes for dye-sensitized solar cells”, Anamaria Trandafir, Adrian Trandafir, C. I. Oprea, M. A. Gîrțu, *Romanian Reports in Physics* **66**, 574-592 (2014)
9. „Disorder, Exchange and Magnetic Anisotropy in the Room-Temperature Molecular Magnet V[TCNE]<sub>x</sub> – A Theoretical Study”, F. Cimpoesu, B. Frecus, C. I. Oprea, P. Panait, M. A. Gîrțu, *Computational Materials Science* **91**, 320-328 (2014)
10. „Ab initio Study of Exchange Coupling for the Consistent Understanding of the Magnetic Ordering at Room-Temperature in V[TCNE]<sub>x</sub>”, B. Frecus, C. I. Oprea, P. Panait, M. Ferbinteanu, F. Cimpoesu, M. A. Gîrțu, *Theoretical Chemistry Accounts* **133** (5), 1470, 1-17 (2014)
11. „Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based Complexes”, C. I. Oprea, P. Panait, B. F. Minaev, H. Agren, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, *Molecular Physics* **111** (8-11, SI), 1526-1538 (2013)
12. „Density Functional Theory (DFT) Study of Coumarin-Based Dyes Adsorbed on TiO<sub>2</sub> Nanoclusters—Applications to Dye-Sensitized Solar Cells”, C. I. Oprea, P. Panait, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, *Materials* **6** (6), 2372-2392 (2013)
13. „New Insights in the Bonding Regime and Ligand Field in Wernerian Complexes. A Density Functional Study”, F. Cimpoesu, A. Zaharia, D. Stamate, P. Panait, C. I. Oprea, M. A. Gîrțu, M. Ferbinteanu, *Polyhedron* **52** (SI), 183-195 (2013)
14. „DFT Study of Binding and Electron Transfer from a Metal-Free Dye with Carboxyl, Hydroxyl, and Sulfonic Anchors to a Titanium Dioxide Nanocluster”, C. I. Oprea, P. Panait, J. Lungu, D. Stamate, A. Dumbravă, F. Cimpoesu, M. A. Gîrțu, *International Journal of Photoenergy*, 893850 (2013)
15. „A Combined Experimental and Theoretical Study of Natural Betalain Pigments Used in Dye-sensitized Solar Cells”, C. I. Oprea, A. Dumbravă, I. Enache, A. Georgescu, M. A. Gîrțu, *Journal of Photochemistry and Photobiology A: Chemistry* **240**, 5-13 (2012)
16. „Broken Symmetry DFT Calculations of Exchange Coupling Constants for Manganese-Porphyrin Quasi-One-Dimensional Molecular Magnets”, C. I. Oprea, P. Panait, F. Cimpoesu, I. Humelnicu, M. Ferbinteanu, M. A. Gîrțu, *Theoretical Chemistry Accounts* **131**, 1249 (2012)
17. „Toward a More Efficient Utilisation of Betalains as Pigments for Dye-Sensitized Solar Cells”, A. Dumbravă, I. Enache, C. I. Oprea, A. Georgescu, M. A. Gîrțu, *Digest Journal of Nanomaterials and Biostructures* **7**, 339-351 (2012)
18. “Role of Energy Level Alignment in Solar Cells Sensitized with a Metal-free Organic Dye - A Combined Experimental and Theoretical Approach”, C. I. Oprea, A. Dumbravă, I. Enache, J. Lungu, A. Georgescu, F. Moscalu, C. Oprea, M. A. Gîrțu, *Physica Status Solidi A-Applications and Materials Science* **208**, 2467-2477 (2011)
19. „DFT Study of Structure-Properties Correlations in [MnTPP][TCNE] Quasi One-Dimensional Molecular Magnets”, C. I. Oprea, F. Cimpoesu, P. Panait, B. Frecus, M. Ferbinteanu, M. A. Gîrțu, *Theoretical Chemistry Accounts* **129**, 847-857 (2011)
20. „DFT Study of Electronic Structure and Optical Properties of Some Ru- and Rh-Based Complexes for Dye-Sensitized Solar Cells”, C. I. Oprea, B. Frecus, B. F. Minaev, M. A. Gîrțu, *Molecular Physics* **109**, 2511-2523 (2011)

21. „DFT Study of the Optical and Vibration Spectra of a Series of Platinum-Olefin Complexes”, C. I. Oprea, F. Moscalu, A. Dumbravă, S. Ioannou, A. Nicolaidis, M. A. Gîțu, *Romanian Journal of Physics* **56**, 1-2, 125-133 (2011)
22. “Heterocyclic Azodyes as Pigments for Dye Sensitized Solar Cells – A Combined Experimental and Theoretical Approach”, J. Lungu, C. I. Oprea, A. Dumbravă, I. Enache, A. Georgescu, C. Rădulescu, I. Ioniță, Gh. V. Cimpoca, M. A. Gîțu, *J. Optoelectr. Adv. Mat.* **12**, 9, 1969-1975 (2010)
23. „Optical and Infrared Properties of a Series of Pyramidalized Olefin Pt-Complexes – DFT Study”, C. I. Oprea, F. Moscalu, A. Dumbravă, S. Ioannou, A. Nicolaidis, M. A. Gîțu, *J. Optoelectr. Adv. Mat.* **11**, 56, 1773-1778 (2009)
24. „Degenerate Perturbation Theory for Electronic g Tensors: Leading-Order Relativistic Effects”, Z. Rinkevicius, K. J. de Almeida, C. I. Oprea, O. Vahtras, K. Ruud, H. Ågren, *J. Chem. Theory and Comput.* **4**, 1810 (2008)
25. “Time-Dependent Density Functional Theory for Non-Linear Properties of Open-Shell Systems”, Z. Rinkevicius, P. C. Jha, C. I. Oprea, O. Vahtras, H. Ågren, *J. Chem. Phys.* **127**, 114101 (2007)
26. “Theoretical Study of Neutral and Reduced Hexacyanobutadiene”, C. I. Oprea, A. Damian, M. A. Gîțu, *J. Mol. Struct.-Theochem* **804**, 111-116 (2007)
27. “Time-Dependent Density Functional Theory with the Generalized Restricted-Unrestricted Approach”, C. I. Oprea, L. Telyatnyk, Z. Rinkevicius, O. Vahtras, H. Ågren, *J. Chem. Phys.* **124**, 174103 (2006)
28. “Spin Density Calculations for Two Electron-Acceptor Constituents of Molecular Magnets: Tetracyanoethylene and Hexacyanobutadiene”, C. I. Oprea, A. Damian, M. A. Gîțu, *J. Optoelectr. Adv. Mat.* **8**, 191-196 (2006)
29. “Density Functional Theory Study of Indirect Nuclear Spin-Spin Coupling Constants with Spin-Orbit Corrections”, C. I. Oprea, Z. Rinkevicius, O. Vahtras, H. Ågren, K. Ruud, *J. Chem. Phys.* **123**, 014101 (2005)

#### Articole publicate în ISI proceedings:

1. “Electron Transfer and Dye Regeneration in Dye-Sensitized Solar Cells”, C. I. Oprea, A. Ndiaye, Anamaria Trandafir, F. Cimpoesu, M. A. Gîțu, *IEEE*, p. 273-276, „2018 International Semiconductor Conference CAS”, Oct 10-12, 2018, Sinaia, Romania, edited by Gh. Brezeanu, M.L. Ciurea, D. Cristea, M.A. Dinescu, D. Dobrescu, M. Dragoman, A. Müller, R. Müller, D. Neculoiu, published by IEEE (2018), DOI: 10.1109/SMICND.2018.8539783, <https://ieeexplore.ieee.org/document/8539783>
2. “DFT Calculations of Structure and Optical Properties in Wide Band-Gap Semiconductor Clusters for Dye-Sensitized Solar Cells”, C. I. Oprea, P. Panait, R. M. Abd El-Aal, M. A. Gîțu, *IEEE*, p. 17-26, „2018 International Semiconductor Conference CAS”, Oct 10-12, 2018, Sinaia, Romania, edited by Gh. Brezeanu, M.L. Ciurea, D. Cristea, M.A. Dinescu, D. Dobrescu, M. Dragoman, A. Müller, R. Müller, D. Neculoiu, published by IEEE (2018), DOI: 10.1109/SMICND.2018.8539813, <https://ieeexplore.ieee.org/document/8539813>
3. „DFT Study of Binding and Electron Transfer from Penicillin to a TiO<sub>2</sub> Nanocluster: Applications to Photocatalytic Degradation”, C. I. Oprea, L. C. Petcu, M. A. Gîțu, *IEEE - 2015 E-HEALTH AND BIOENGINEERING CONFERENCE (EHB)*, „5<sup>th</sup> IEEE International Conference on E-Health and Bioengineering, Nov. 19-21, 2015, Iași, Romania”, edited by H. N. Costin, published by IEEE (2015)
4. „DFT Study of Optical Properties of Pt-based Complexes”, C. I. Oprea, A. Dumbravă, F. Moscalu, A. Nicolaidis, M. A. Gîțu, *AIP CP1203*, 1198-1203, „7<sup>th</sup> International Conference of the Balkan Physical Union”, edited by A. Angelopoulos and T. Fildisis, published by American Institute of Physics, 1198 (2009)
5. “Theoretical Calculations of Structure and Exchange Coupling of a Room-Temperature Molecular Magnet”, F. Cimpoesu, B. Frecuș, C. I. Oprea, M. A. Gîțu, *AIP CP1203*, 1192-1197, „7<sup>th</sup> International Conference of the Balkan Physical Union”, edited by A. Angelopoulos and T. Fildisis, published by American Institute of Physics, 1198 (2009)
6. “DFT Calculations of a Metal-TCNE Complex”, C. I. Oprea, A. Damian, M. A. Gîțu, „Sixth International Conference of the Balkan Physical Union”, edited by S.A. Cetin and I. Hikmet, published by American Institute of Physics, 716 (2007)

#### Articole publicate în alte jurnale:

1. “Assesing Quantum Calculation Methods for the Account of Ligand Field in Lanthanide Compounds”, A. M. Toader, B. Frecuș, C. I. Oprea, M. C. Buta, *Physchem* **3** (2), 270-289 (2023)
2. „DFT Calculations of Ru- and Rh-based Complexes for Dye-Sensitized Solar Cells”, C. I. Oprea, B. Frecuș, B. F. Minaev, M. A. Gîțu, *Вісник Черкаського університету, Серія «Хімічні науки»* **175**, 106-111 (2010), [www.nbu.gov.ua/Portal/Soc\\_Gum/Vchu/N175/N175p106-111.pdf](http://www.nbu.gov.ua/Portal/Soc_Gum/Vchu/N175/N175p106-111.pdf)
3. “The Influence of Spin-orbit Coupling on Ferromagnetism”, C. I. Oprea, , *Ovidius Univ. Ann. Phys.* **3**, 91-96 (2002)
4. “Renormalization Approach to 1-D Potts Model”, C. I. Oprea, , *Ovidius Univ. Ann. Phys.* **2**, 89-94 (2001)

#### Articole publicate în alte proceedings:

1. „New Mixed Ligand Co(II) Complexes as Possible Electrolytes for Dye-Sensitized Solar Cells – A Combined Experimental and Theoretical Approach”, D. Stamate, M. Ferbinteanu, C. I. Oprea, P. Panait, F. Cimpoesu, M. A. Gîțu, *1<sup>st</sup> International Electronic Conference on Materials*, 26 May-10 June, 2014, <https://sciforum.net/paper/view/conference/2365> , DOI 10.3390/ecm-1-b003
2. “Ab Initio Study of Electron Acceptor Molecules for Organic Electronics and Molecular Magnetism”, C. I. Oprea, B. Frecuș, F. Moscalu, M. A. Gîțu, “Proceedings of the Nano-Sol-Net International Symposium: Trends in Organic Electronics and Hybrid Photovoltaics”, edited by M. A. Gîțu and M. Fahlman, Ovidius University Press, Constanța 2008, ISBN 978-973-614-414-1, pp. 69-75
3. “Quantum Chemical Calculations of Three Electron-Acceptor Molecules: TCNE, TCNQ and HCB<sup>D</sup>”, C. I. Oprea, I. Carazeanu-Popovici, M. A. Gîțu, *Bulletin of the Transilvania University of Brașov (BRAMAT)* **3**, 409-414 (2007)

4. "Density Functional Theory Calculations of Electron Affinities and Spin Densities of Two Electron-Acceptor Molecules", A. Damian, C. I. Oprea, M. A. Gîrțu, "Convergence of micro-nano-biotechnologies" în seria "Micro and Nanoengineering", vol. 9, Ed. Academiei, Bucuresti (2006), ISBN (10) 973-27-1422-0 și ISBN (13) 978-973-27-1422-5, pp. 9-15

#### **Cărți:**

1. "Optica. Îndrumar de laborator – partea I", Mihai A. Gîrțu and Corneliu I. Oprea, Editura Ovidius University Press, Constanța 2008, ISBN 978-973-614-413-4

#### **Capitole în cărți:**

1. „Room Temperature Molecular Magnets: Modeling and Applications”, Mihai A. Gîrțu and Corneliu I. Oprea, in Advanced Magnetic and Optical Materials, ed. by Ashutosh Tiwari et al., co-published by John Wiley & Sons, Beverly, MA, and Scrivener Publishing, Hoboken, NJ, USA 2017, ISBN 978-1-119-24191-1

#### **Lecții Invitate:**

1. „TiO<sub>2</sub> Photocatalytic Degradation of Common Antibiotics – A DFT Study”, C. I. Oprea, M. A. Gîrțu, 16<sup>th</sup> International Balkan Workshop on Applied Physics, July 7-9, 2016, Constanța, Romania
2. „A Computational Study of Dye Regeneration by Cobalt-Based Electrolytes – Applications to Dye-Sensitized Solar Cells”, C. I. Oprea, Anamaria Trandafir, Adrian Trandafir, P. Panait, D. Stamate, M. Ferbinteanu, F. Cimpoesu, M. A. Gîrțu, 14<sup>th</sup> International Balkan Workshop on Applied Physics, July 2-4, 2014, Constanța, Romania
3. „Magnetic Ordering in a Family of High Temperature Molecular Magnets – A Computational Approach”, C. I. Oprea, P. Panait, B. Frecus, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, 13<sup>th</sup> International Balkan Workshop on Applied Physics, July 4-6, 2013, Constanța, Romania
4. "Density Functional Theory Applied to Electron and Nuclear Magnetic Resonance", C. I. Oprea, 8<sup>th</sup> International Balkan Workshop on Applied Physics, July 5-7, 2007, Constanța, Romania

#### **Prezentări orale la conferințe:**

1. „A Computational Study of Coumarin-Based Dyes Adsorbed on TiO<sub>2</sub> Nanoclusters – Applications to Dye-Sensitized Solar Cells”, C. I. Oprea, P. Panait, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, 13<sup>th</sup> International Balkan Workshop on Applied Physics, July 4-6, 2013, Constanța, Romania
2. „Hybrid Organic-Inorganic Solar Cells - A Computational Study of Coumarin Dyes Adsorbed on Titania Nanoclusters”, C. I. Oprea, P. Panait, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, Nav-Mar-Edu 2013, May 30 – June 1, 2013, Constanta, Romania
3. "Structure-properties Correlations for Three Manganese-porphyrin Quasi-one-dimensional Molecular Magnets", C. I. Oprea, P. Panait, F. Cimpoesu, I. Humelnicu, M. Ferbinteanu, M. A. Gîrțu, Physics Conference TIM12, Nov. 27-30, 2012, Timisoara, Romania
4. "Magnetic or Optical Properties of Systems Based on Transition Metal Complexes with Porphyrin and Bipyridine Ligands", C. I. Oprea, P. Panait, B. Frecus, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, Advanced Structure-Property Correlation, the Gate for Special Properties at Molecular and Nano Level, ADSPECPRO 2012, Sept. 20-21, 2012, Bucharest, Romania
5. "Metal-free Pigments for Dye Sensitized Solar Cells - A Combined Experimental and Theoretical Approach", C. I. Oprea, A. Dumbravă, J. Lungu, I. Enache, A. Georgescu, C. Oprea, F. Moscalu, M. A. Gîrțu, 27<sup>th</sup> International Congress of the Turkish Physical Society, Sept 14-17, 2010, Istanbul, Turkey
6. "Density Functional Theory Calculations of TiO<sub>2</sub> Anatase Nanoparticles", C. I. Oprea, P. Panait, B. Frecuș, F. Moscalu, V. Pomazan, F. Cimpoesu, M. A. Gîrțu, 19<sup>th</sup> International Workshop on Computational Mechanics of Materials, Sept. 1-4, 2009, Constanța, Romania
7. "Relativistic Effects on EPR g-tensors", C. I. Oprea, NANOQUANT Young Researchers Meeting, Dec. 9, 2006, Tartu, Estonia

#### **Seminarii științifice:**

1. "Role of energy level alignment in solar cells sensitized with organic and organometallic dyes", C. I. Oprea, Department of Theoretical Chemistry and Biology, School of Biotechnology, Royal Institute of Technology, Stockholm, Suedia, Aug. 26, 2011, grant PN2-RU-PD-603 nr. 117/2010
2. "Quantum Chemical Study of an Organic Dye for DSSCs", C. I. Oprea, Cherkassy, Ukraine, Oct. 22, 2009, grant PN2-Capacități-M3 nr. 116/2008
3. "Quantum Chemical Study of Optical Properties of Organic Dyes and Pt-Based Complexes", C. I. Oprea, Nicosia, Cyprus, Sept. 10, 2009, grant PN2-Capacități-M3 nr. 128/2008
4. "Quantum Chemical Calculations of Dye-Sensitized Solar Cells on TiO<sub>2</sub> Substrate", C. I. Oprea, Cherkassy, Ukraine, Oct. 16, 2008, grant PN2-Capacități-M3 nr. 116/2008
5. "Density Functional Theory Studies of Relativistic Magnetic Resonance Parameters", C. I. Oprea, NANOQUANT Midterm Meeting, Feb. 10-11, 2006, Oslo, Norway

#### **Postere:**

1. „Modeling TiO<sub>2</sub> Nanoclusters for Photocatalytic Degradation of Penicillins”, C. I. Oprea, P. Panait, M. A. Gîrțu, F. Cimpoesu, 20<sup>th</sup> International Balkan Workshop on Applied Physics, July 12-15, 2022, Constanța, Romania

2. „First-principle Studies of Charge Transfer in Model Systems Representative for Dye-Sensitized Solar Cells”, C. I. Oprea, A. M. Toader, F. Cimpoesu, A. Ndiaye, M. A. Gîrțu, 19<sup>th</sup> International Balkan Workshop on Applied Physics, July 17-19, 2019, Constanța, Romania
3. „Modeling Molecules Interacting with TiO<sub>2</sub> Nanoclusters for Hybrid Organic-inorganic Photovoltaics or Photocatalytic Degradation of Pollutants”, C. I. Oprea, M. A. Gîrțu, Physics Conference TIM-19, May 29-31, 2019, Timișoara, Romania
4. “Electron Transfer and Dye Regeneration in Dye-Sensitized Solar Cells”, C. I. Oprea, A. Ndiaye, Anamaria Trandafir, F. Cimpoesu, M. A. Gîrțu, International Semiconductor Conference CAS 2018, Oct 10-12, 2018, Sinaia, Romania
5. „DFT Study of Coumarin-Based Dyes Adsorbed on TiO<sub>2</sub> Nanoclusters — Applications to Dye-Sensitized Solar Cells”, C. I. Oprea, P. Panait, F. Cimpoesu, M. Ferbinteanu, M. A. Gîrțu, 7<sup>th</sup> Molecular Quantum Mechanics MQM 2013, June 2-7, 2013, Lugano, Switzerland
6. “Quantum Chemical Study of Optical Properties of Some Ru- and Rh-Based Complexes for Dye-Sensitized Solar Cells”, C. I. Oprea, P. Panait, B. F. Minaev, M. A. Gîrțu, 5<sup>th</sup> International Conference on Molecular Materials MOLMAT 2012, July 3-6, 2012, Barcelona, Spain
7. “Role of Energy Level Alignment in Solar Cells Sensitized with a Metal-free Organic Dye: A Combined Experimental and Theoretical Approach”, C. I. Oprea, A. Dumbravă, I. Enache, J. Lungu, A. Georgescu, C. Oprea, F. Moscalu, M. A. Gîrțu, European Congress and Exhibition on Advanced Materials and Processes EUROMAT 2011, Sept. 12-15, 2011, Montpellier, France
8. “Role of Energy Level Alignment in Dye Sensitized Solar Cells – A Case Study on Mordant Yellow-10”, A. Dumbravă, C. I. Oprea, I. Enache, J. Lungu, A. Georgescu, C. Oprea, F. Moscalu, M. A. Gîrțu, 12<sup>th</sup> International Balkan Workshop on Applied Physics, July 6-8, 2011, Constanța, Romania
9. “Broken Symmetry DFT Calculations of Exchange Interactions in Mn-Porphyrin Molecular Magnets”, C. I. Oprea, P. Panait, B. Frecuș, F. Cimpoesu, M. A. Gîrțu, Physics Conference TIM-10, Nov. 25-27, 2010, Timișoara, Romania
10. “Mordant Yellow-10 as a Pigment for Dye Sensitized Solar Cells - Experimental and Theoretical Approach”, C. I. Oprea, A. Dumbravă, J. Lungu, I. Enache, A. Georgescu, C. Oprea, F. Moscalu, M. A. Gîrțu, Conferința Națională de Fizică, 23-25 sept 2010, Iași, Romania
11. “DFT Study of Optical Properties of Organic Dyes and Pt-Based Complexes”, C. I. Oprea, F. Moscalu, A. Dumbravă, A. Nicolaidis, M. A. Gîrțu, 10<sup>th</sup> International Balkan Workshop on Applied Physics, July 6-8, 2009, Constanța, Romania
12. “Ru- and Rh-Based Complexes as Pigments for Dye-Sensitized Solar Cells – A DFT Study”, C. I. Oprea, B. Frecuș, P. Panait, F. Moscalu, A. Dumbravă, B. F. Minaev, M. A. Gîrțu, 10<sup>th</sup> International Balkan Workshop on Applied Physics, July 6-8, 2009, Constanța, Romania
13. “DFT Study of Ru- and Rh-Based Complexes as Pigments for Dye-Sensitized Solar Cells”, C. I. Oprea, B. Frecuș, P. Panait, F. Moscalu, A. Dumbravă, M. A. Gîrțu, International Conference Chimia 2009 „New Trends in Applied Chemistry”, May 13-16, 2009, Constanța, Romania
14. “Ab Initio Study of Electron Acceptor Molecules for Organic Electronics and Molecular Magnetism”, C. I. Oprea, B. Frecuș, F. Moscalu, M. A. Gîrțu, Nano-Sol-Net International Symposium: Trends in Organic Electronics and Hybrid Photovoltaics, June 12-14, 2008, Eforie Nord, Romania
15. “DFT Calculations of Metal-TCNE Complexes as Models for M[TCNE]<sub>2</sub> Magnets”, C. I. Oprea, G. Damache, A. Georgescu, M. A. Gîrțu, 5<sup>th</sup> International Conference „New research trends in materials science” ARM-5, Sept. 5-7, 2007, Sibiu, Romania
16. “DFT Study of Electron-Acceptor Molecules – Comparison Between TCNE, TCNQ, and HCBd”, C. I. Oprea, F. Moscalu, M. A. Gîrțu, 8<sup>th</sup> International Balkan Workshop on Applied Physics, July 5-7, 2007, Constanța, Romania
17. “Density Functional Theory with the Restricted-Unrestricted Approach”, C. I. Oprea, L. Telyatnyk, Z. Rinkevicius, O. Vahtras, 6<sup>th</sup> Svensk Teoretisk Kemi Conference, May 4-5, 2006, Stockholm, Suedia

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## LISTA GRANTURILOR DE CECETARE

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### Grant național ca director:

1. 2010-2012, PN-II-RU-PD-603 „Molecular Modeling of Pigments for Dye-sensitized Solar Cells by Density Functional Methods”

### Granturi Internaționale ca membru în echipă:

1. 2012-2014, Romania-Switzerland Research Programme (RSRP # IZERO-142144/1), PN-II-Idei-RSRP 1: “Development of Novel Materials for High Efficiency Dye-Sensitized Solar Cells”, principal investigators: Prof. Mihai A. Gîrțu, „Ovidius” University of Constanța and Michael Grätzel, Ecole Polytechnique Fédérale de Lausanne
2. 2008-2009, PN-II-Capacități-M3-128 bilateral Cyprus-Romania research project “Towards New Photovoltaic Materials: Calculations, Synthesis and Measurements”, principal investigators: Prof. Mihai A. Gîrțu, „Ovidius” University of Constanța and Prof. Athanassios Nicolaidis, University of Cyprus, Nicosia
3. 2008-2009, PN-II-Capacități-M3-116 bilateral Ukraine-Romania, research project „Design of Novel Sensitizing Dyes for Nanocrystalline TiO<sub>2</sub> Solar Cells on the Basis of Their Electronic Structure Calculations”, principal investigators: Prof. Mihai A. Gîrțu, „Ovidius” University of Constanța and Prof. Boris F. Minaev, Cherkassy Engineering and Technological Institute
4. 2004-2007, Marie Curie RTN – NANOQUANT “Understanding Nano-materials from the Quantum perspective”, principal investigator: Prof. Hans Agren, Royal Institute of Technology, Stockholm, Suedia

### Granturi naționale ca membru în echipă:

1. 2022-2024, PN-III-P4-PCE-2021-1881 „New Advances in Theoretical Understanding of Rare-Earth Emission. Fundamentals for Applications by Rational Property Design”, principal investigator: Senior researcher Fănică Cimpoeșu, „I.G. Murgulescu” Institute for Physical Chemistry, Bucharest
2. 2017-2019, PN-III-P4-ID-PCE-2016-0689 „Analize critice si dezvoltari teoretice fundamentale in chimia computationally”, principal investigator: Senior researcher Fănică Cimpoeșu, „I.G. Murgulescu” Institute for Physical Chemistry, Bucharest
3. 2014-2015, PN-II-ID-PCE-14/2013 „Methodological Advances and Theoretical Experiments on the Bonding Regime and Properties Design. From atoms to Supra-molecules”, principal investigator: Senior researcher Fănică Cimpoeșu, „I.G. Murgulescu” Institute for Physical Chemistry, Bucharest
4. 2015-2016, Scientific projects “Small Angle Neutron Scattering Investigations of the Nanocrystalline Wide Band Gap Semiconductors for Dye-Sensitized Solar Cells and Photocatalytical Applications”, principal investigator Assist. prof. Florin Moscalu, „Ovidius” University of Constanța and “Microstructure Investigation of Materials Based on Carbon at Nanoscale by Means of Small Angle Scattering”, principal investigator Assoc. prof. Rodica Vlădoiu, „Ovidius” University of Constanța, part of Romania-IUCN Cooperation Protocol No. 4405-4-2015/2017, Topic No. 04-4-1121-2015/2017; 2019, Project No. 91, JINR-RO 2018, topic number 04-4-1121-2015/2020, JINR 322/21.05.2018, Dubna, Russia, „Composite materials based on inorganic semiconductors for photovoltaic cells and photocatalytic applications” principal investigator Assist. prof. Florin Moscalu, „Ovidius” University of Constanța
5. 2010-2013, PN-II-ID-PCCE-239 „A New Generation of Paradigms in Molecular Magnetism and Materials Science, Magnetic Anisotropy in Complex Units, Supramolecular Systems and at Nanoscale”, principal investigators: Prof. Marilena Ferbințeanu-Cimpoeșu, University of Bucharest and Prof. Mihai A. Gîrțu, „Ovidius” University of Constanța

### Proiecte de infrastructură ca membru în echipă:

1. 2020-2022, Proiect POCU/864/6/21/140783 din 09.12.2020, “Start în carieră prin masterat didactic”, responsabil Conf. univ. dr. Cristian Petre, Universitatea Ovidius din Constanța
2. 2020-2022, Proiect privind învățământul secundar, acord de grant ROSE-258/SGU/NC/II din 25.11.2019, “Antrenare, Coordonare, Consiliere și Educație în timpul Studenției ACCES”, director Prof. univ. dr. Rodica Vlădoiu, Universitatea Ovidius din Constanța
3. 2019, contract CNFIS-FDI-2019-0558, D6 - Susținerea cercetării de excelență din universități, „Excelență, performanță și competitivitate în cercetarea biomedicală din Universitatea „Ovidius” din Constanța”, director Conf. univ. dr. Irina Magdalena Dumitru, Universitatea Ovidius din Constanța
4. 2014-2015, contract POSDRU/156/1.2/G/136858, “MATE-INFO.NET, Adaptarea programelor de studii universitare la Cadrul Național al Calificărilor în Învățământul Superior și crearea unei rețele virtuale în vederea îmbunătățirii interacțiunii cu mediul de afaceri pentru a susține dezvoltarea economică și socială”, director Lect. univ. dr. Alexandru Bobe, Universitatea Ovidius din Constanța

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