



## INFORMAȚII PERSONALE



## Călin Gabriel Floare

 Institutul Național de Cercetare-Dezvoltare pentru Tehnologii Izotopice și Moleculare, Cluj-Napoca, România

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Sexul Masculin | Data nașterii 09/02/1973 | Naționalitatea română

## EXPERIENȚA PROFESIONALĂ

10/1997–Prezent

**Cercetător Științific III**

National Institute for R & D of Isotopic and Molecular Technologies (Cluj-Napoca, Romania)

Supervizor: Dr. Adrian Pamula and Dr. Mircea Bogdan

- Asistent cercetare în Laboratorul de Spectrometrie de Masă
- Cercetător Științific III în Grupul de Rezonanță Magnetică Nucleară

09/2007–07/2008

**Profesor asistent (secția de limbă franceză)**

Departamentul de Biofizică al Universității de Medicină și Farmacie "Iuliu Hațieganu", Cluj-Napoca (România)

Supervizor: Prof. Constantin Mihai Lucaciu

## EDUCAȚIE ȘI FORMARE

06/2014–06/2016

**Master în Biotehnologii Moleculare**

Universitatea Babeș-Bolyai, Facultatea de Biologie-Geologie (Cluj-Napoca, Romania)

Titlul lucrării de disertație : Obținerea feredoxinei recombinate de la *Streptomyces Griseolus*

Supervizor: Prof. dr. Iulia Lupan

06/2000–11/2005

**Doctorat în Fizică**

Universitatea Joseph Fourier, Grenoble (France)

Titlul tezei : Dinamică și reactivitate în medii restrânse

Supervizor: Prof. Hans Peter Trommsdorff și Prof. Simion Astilean

<https://tel.archives-ouvertes.fr/tel-00011550/>

10/1997 - 06/1998

**Master în Fizică Teoretică**

Universitatea Babeș-Bolyai, Facultatea de Fizică (Cluj-Napoca, Romania)

Titlul lucrării de disertație : Dinamică moleculară 'tight-binding' pentru molecula de fulerenă (C<sub>60</sub>)

Supervizor: Prof. Titus Adrian Beu

10/1991 - 06/1997

**Licențiat în Fizică Tehnologică – Titlul: Inginer Fizician**

Universitatea Babeș-Bolyai, Facultatea de Fizică (Cluj-Napoca, Romania)

Titlul lucrării de diplomă : Clusteri moleculari SF<sub>6</sub> – Ar

Supervizor: Prof. Titus Adrian Beu

STAGII DE CERCETARE

2/10/2021 - 30/11/2021  
 30/09/2019 - 1/10/2019  
 1/10/2012 - 8/12/2012  
 28/06/2011 - 9/07/2011

Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italia

'Statistical and Biological Physics', Supervisor: Prof. Alessandro Laio

<http://www.sissa.it/>

July 9 - 28, 2011

▪ În cadrul proiectelor HPC-Europa 2 & 3 - <http://www.hpc-europa.eu/>  
**CINECA, Bologna, Italia**

<http://www.cineca.it/>

05/2003 - 08/2003  
 11/2001 - 05/2002

▪ În cadrul proiectului HPC-Europa 2 - <http://www.hpc-europa.eu/>  
**Institututul Laue-Langevin, Grenoble, Franța**

<http://www.ill.eu/instruments-support/computing-for-science/home/>

Grupul 'Computing for Science', Supervisor: Dr. Mark Johnson

▪ Student Doctorand

COMPETENȚE PERSONALE

Limba(i) maternă(e)

română

Alte limbi străine cunoscute

	ÎNȚELEGERE		VORBIRE		SCRIERE
	Ascultare	Citare	Participare la conversație	Discurs oral	
engleză	B2	B2	B2	B2	B2
franceză	B2	B2	B2	B2	B2

Niveluri: A1 și A2: Utilizator elementar - B1 și B2: Utilizator independent - C1 și C2: Utilizator experimentat  
 Cadrul european comun de referință pentru limbi străine

Competențe de comunicare

Abilitatea de a interacționa și de a comunica eficient cu oameni din diverse medii, evidențiind munca în echipă și rezolvarea problemelor

Competențe organizaționale/manageriale

Director al unui proiect de cercetare național și a două proiecte în cadrul HPC-Europa 2 & 3

Competențe dobândite la locul de muncă

- spectroscopie de rezonanță magnetică nucleară, spectrometrie de masă, spectroscopie de absorbție UV-vis, vibrațională (în infraroșu și Raman), spectroscopie de fluorescență, metode de biologie și biotehnologie moleculară, împrăștiere dinamică a luminii, calorimetrie de scanare diferențială
- chimie și biochimie computațională: calcule ab initio, dinamică moleculară, andocare moleculară
- dezvoltare software: C, C++, Fortran, Python, TCL, Octave, Matlab, MPI, CUDA
- administrare cluster Linux de înaltă performanță: Torque, Maui, Ganglia, Nagios, IBM LSF & GPFS

Competență digitală

AUTOEVALUARE				
Procesarea informației	Comunicare	Creare de conținut	Securitate	Rezolvarea de probleme
Utilizator experimentat	Utilizator experimentat	Utilizator experimentat	Utilizator experimentat	Utilizator experimentat

Competențele digitale - Grilă de auto-evaluare

Permis de conducere

Categoria B

## INFORMAȚII SUPLIMENTARE

## Publicații

[Brainmap](#) [Google Scholar](#) [ORCID](#) [Scopus](#) [Web of Science](#)

- **C.G. Floare**, M. Bogdan, Maria Tomoaia-Cotisel and Aurora Mocanu, <sup>1</sup>H NMR spectroscopic characterization of inclusion complex of desferrioxamine B chelator and β-cyclodextrin, *J. Mol. Struct.* 1248, 131477 (2022)
  - Mihaela Mic, A. Pîrnau, **C. G. Floare**, G. Marc, Ana H. Franchini, O. Oniga, L. Vlase and M. Bogdan, Synthesis and molecular interaction study of a diphenolic hidrazinyl-thiazole compound with strong antioxidant and antiradical activity with HSA, *J. Mol. Struct.* 1244, 131278 (2021)
  - Mihaela Mic, A. Pîrnau, **C. G. Floare** and M. Bogdan Study of the binding affinity between imatinib and alpha-1 glycoprotein using nuclear spin relaxation and isothermal titration calorimetry, *Int. J. of Biol. Macromolec.* 147, 326-332 (2020)
  - A. Pîrnau, Mihaela Mic, Silvia Neamtu, **C.G. Floare** and M. Bogdan, Calorimetric and spectroscopic studies of the interaction between zidovudine and human serum albumin, *Spectrochim. Acta A - Molec. and Biomolec. Spectrosc.* 191, 226-232 (2018)
  - Mihaela Mic, A. Pîrnau, **C.G. Floare**, Maria Miclaus, Irina Kacso, Mariana Palage and M. Bogdan, Interaction of 1-methyl-1-({2-[4-(trifluoromethyl)phenyl]-1,3-thiazol-4-yl}methyl) piperidinium chloride with β-CD: spectroscopic, calorimetric and molecular modeling approaches, *J. Incl. Phenom. Macrocycl. Chem.* 92(1-2), 195-204 (2018)
  - A. Farcas, L. Buimaga-larinca, **C.G. Floare**, L. Janosi, Influence of G12V mutation on NRas proteins' aggregation, *European Biophysics Journal with Biophysics Letters* 46(1), S399-S399, P-1080 (2017)
  - L. Janosi, **C. G. Floare**, A. Farcas, L. Buimaga-larinca, In silico study of Ras-binding peptides' self-association, 19th IUPAB Congress / 11th EBSA Congress, *European Biophysics Journal with Biophysics Letters* 46(1), S398-S398, P-1081 (2017)
  - M. Bogdan, **C.G. Floare**, A. Pîrnău, S. Neamtu, Competitive Binding of Tolmetin to beta-Cyclodextrin and Human Serum Albumin: H-1 NMR and Fluorescence Spectroscopy Studies, *J. Sol. Chem.* 46(1), 44-57 (2017)
  - D.I. Bilc, **C.G. Floare**, L.P. Zarbo, S. Garabagiu, S. Lemal, P. Ghosez, First-Principles Modeling of SrTiO<sub>3</sub> Based Oxides for Thermoelectric Applications, *J. Phys. Chem. C* 120(45) 25678-25688 (2016)
  - Alexandra Farcaș, Luiza Buimaga-larinca, **C.G. Floare**, L. Janosi, Mammalian membrane model behavior in the presence of Ras protein nanoclusters, *FEBS JOURNAL* 283 SI(1), 236 (2016)
  - M. Bogdan, **C.G. Floare**, Luiza Buimaga-larinca, C. Morari, A. Pîrnau, NMR study and computational assays of meclofenamic Na salt and β-cyclodextrin inclusion complex, *J. Incl. Phenom. Macrocycl. Chem.* 85(1), 111-120 (2016)
  - Luiza Buimaga-larinca, **C.G. Floare**, C. Morari, DFT study of the trioxotriangulene derivatives in bulk state, *Chem. Phys. Lett.* 598, 48-62 (2014)
  - A. Pîrnău, **C.G. Floare**, M. Bogdan, The Complexation of Flurbiprofen with β-cyclodextrin: a NMR study in aqueous solution, *J. Incl. Phenom. Macrocycl. Chem.* 78 (1-4), 113-120 (2014)
  - **C.G. Floare**, A. Pîrnău, M. Bogdan, <sup>1</sup>H NMR spectroscopic characterization of inclusion complexes of tolfenamic and flufenamic acids with β-cyclodextrin, *J. Mol. Struct.* 1044, 72-78 (2013)
  - **C.G. Floare**, M. Bogdan, CONSTEQ - A program for association constants determination using solution NMR data, *AIP Conference Proceedings*, 1565, 48-52 (2013)
  - **C.G. Floare**, A. Rodriguez and A. Laio, Molecular dynamics investigation of an inverse freezing counterintuitive phenomenon, *HPC-Europa2 - Project Report* (2012)
  - **C.G. Floare**, M. Bogdan, O. Horovitz, A. Mocanu and M. Tomoaia-Cotisel, Analysis of the secondary structure of a protein's N-terminal, *J. of Phys.: Conf. Series* 182, 012008 (2009)
  - A. Pîrnău, M. Bogdan and **C.G. Floare**, NMR spectroscopic characterization of β-cyclodextrin inclusion complex with vanillin, *J. of Phys.: Conf. Series* 182, 012013 (2009)
  - M. Bogdan, **C.G. Floare** and A. Pîrnău, <sup>1</sup>H NMR investigation of self-association of vanillin in aqueous solution, *J. of Phys.: Conf. Series* 182, 012002 (2009)
  - Assa Aravindh et al., Si<sub>x</sub>C<sub>1-x</sub>O<sub>2</sub> alloys: A possible route to stabilize carbon-based silica-like solids?, *Solid State Communications*, 144, 273-276 (2007)
  - M. Bogdan, A. Pîrnău, **C. Floare** and Carmen Bugeac, Binding interaction of indomethacin with human serum albumin, *J. Pharm. Biomed. Anal.*, 47(4-5), 981 (2008)
  - **C. Floare**, S. Astilean, M. Bogdan, O. Cozar, DFT Structure Optimization and Vibrational Spectra of the Photochromic 2-(2',4'-dinitrobenzyl)pyridine, *Rom. J. Phys.*, 50 (7-8), 815 (2005)
  - **C. Floare**, S. Astilean, M. Bogdan, O. Cozar, Drastic influence of β-Cyclodextrin on the anionic α-DNBP in DMSO solution, *Advanced Spectroscopies on Biomedical and Nanostructured Systems*, September 19-22, 2004, Cluj-Napoca, Romania (publ. in *Studia Universitatis Babeș-Bolyai, Physica*)
  - M. Plazanet, **C. Floare**, M. R. Johnson, R. Schweins, H. P. Tommsdorff, Freezing on heating of liquid solutions, *J. Chem. Phys.*, 121(11), 5031 (2004) & *ILL Annual Report 2004*, 54-55
- 25 articole ISI, H-Index: 7 în Publons/218 citări, 8 în Scopus/247 citări

## Prezentări Orale

- The 6th International Conference "Distributed Computing and Grid-technologies in Science and Education" (LIT Joint Institute for Nuclear Research, Dubna, Russia) - 30/06/2014 - 5/07/2014 <http://indico-new.jinr.ru/contributionDisplay.py?contribId=20&sessionId=4&confId=19>
- ComplexHPC Spring School 2011 - HPDC Middleware, Environments, and Tools, May 9-13, 2011 (VU University, Amsterdam, The Netherlands): Molecular Dynamics Investigation of an Inverse Freezing Counterintuitive Phenomenon <http://www.cs.vu.nl/complexhpc2011/challenge.html>
- Conference for Young Scientists in Ceramics (SM-2013) and The Third ESR Workshop, (COST MP0904), November 6-9, 2013 (Novi Sad, Serbia): First-principles modelling of SrTiO<sub>3</sub> based oxides for thermoelectric applications
- Cyclodextrin inclusion compounds. Investigation of an unusual phase transition, Scuola Internazionale di Studi Avanzati (SISSA), Trieste, Italy, 24 October 2012 <http://www.sissa.it/sbp/activity/seminarlist.php?show=SBPGS>
- Experimental and theoretical analysis of the encapsulation in cyclodextrins and self-association of Vanillin, 3rd Romanian-South African Symposium "Cyclodextrin Inclusion Complexes", October 9-14, 2010, Moeciu, Romania <http://www.itim-cj.ro/hgcomp/results.html>
- Advances in Computational Studies of Molecular Inclusion Compounds and Proteins, 2nd Romanian-South African Symposium "Cyclodextrin Inclusion Complexes", September 18-23, 2009, Sovata, Romania
- Low field NMR investigation of an unusual phase transition, 1st Romanian-South African Symposium "Cyclodextrin Inclusion Complexes", October 13-14, 2008 INCDTIM Cluj-Napoca, Romania

## Proiecte

**Director de Proiect**

- HPC-Europa 2 &3 - Molecular dynamics investigation of an inverse freezing counterintuitive phenomenon (2012 and 2019).
- CEEEX ET-58/18.09.2006 – Investigare experimentală, ab initio și prin dinamică moleculară a unei tranziții de fază neobișnuite, Valoare totală proiect: 144000 RON

**Membru al echipelor de cercetare**

- Control of electronic properties of heterostructures based on ferroelectric perovskites: from theory to applications, Project Code: PCCF PN-III-P4-ID-PCCF-2016-0047, Contract No.: 16/2018
- Design of Highly Efficient Antimicrobial Peptides: *in silico* prediction and experimental validation, Project Code: PN-III-P1-1.1-TE-2016-0032, Contract no.: 99/2018 <https://www.itim-cj.ro/PNCIDI/te99/>
- Design of some spin-crossover supramolecular structures controlled by ultrashort laser, Project Code: PN-III-P4-ID-PCE-2016-0208, Contract no.: 64/2017 <https://www.itim-cj.ro/pncdi/lascro/>
- High Performance Materials for the next generation Space Thermoelectric Generators, Project Code: PNCIDI-III-C3-2016 STAR, Contract no.: 193/2017 <https://www.itim-cj.ro/pncdi/matspaceteg/>
- Design of New Lipid-Modified peptides to Destabilize Ras Nanoclusters - A therapeutic approach for targeting oncogenic RAS proteins, Project Code: PN-II-RU-TE-2014-4-2418, Contract No.: 118/01.10.2015, Total project value: 549,146 RON <http://www.itim-cj.ro/PNCIDI/ru118/>
- Bioligand-macromolecule intermolecular interactions studied by spectroscopic and calorimetric techniques, Project code: PN-II-ID-PCE-2011-3-0032, Contract No.: 8/05.10.2011, Total project value: 1,499,400 RON <http://www.itim-cj.ro/PNCIDI/idei8/>
- First Principles Modelling of SrTiO<sub>3</sub> based Oxides for Thermoelectric Applications, Project Code: PN-II-RU-TE-2011-3-0085, Contract No.: 87/05.10.2011, 10.2011-10.2014, Total project value: 919,100 RON <http://www.itim-cj.ro/PNCIDI/ru87/>
- Modern high-throughput methodologies for obtaining and characterizing new solid forms of pharmaceutical compounds, Project code: POSCCE ID 536 / SMIS CSNR 12011, Total project value: 6,604,960 RON <http://www.itim-cj.ro/pos/htpharma/>
- Structure, Physicochemical Properties and Molecular Modeling Studies of "Host-Guest" Type Inclusion Complexes (HGCOMP), 05/2008-12/2010, Joint Research Project under the Romania-South Africa Agreement on Cooperation in Science and Technology, Prof Mino R Caira Dept. Chemistry Univ. Cape Town South Africa, 05/2008-12/2010, Total Project Value: 220,756.38 RON <http://www.itim-cj.ro/hgcomp/>
- PN-II-PT-PCCA-2011-3.2-0210 PETOP 169/2012 Petabyte Optical Disc (2012-2016)
- CEEEX-M1-C2-1967 MATNANTECH 58/2006 Molecular Dynamics in polymeric nanocapsules. Investigations using nuclear magnetic resonance (2006-2008)
- CEEEX PC-D01-PT15-137 CALIMED Polymorphic forms and encapsulation of bioactive substances in cyclodextrins to improve the drug quality <http://www.itim-cj.ro/PNCIDI/calimed> (2005-2008)
- CERES 4-36/2004 Unconventional aspects and principles of NMR diffusometry in confined liquids (2004-2006)

## Școli și Workshop-uri

- CASTEP Training Workshop 2019 (Oxford University) - August 19 - 23, 2019 <http://www.castep.org/CASTEP/Workshop2019>
- Advanced Isotopic Labelling Methods for Integrated Structural Biology (IBS, Grenoble, France) – March 26 - April 5 2019 <http://www.aim2019.org>
- Winter College on Optics. Applied Optical Techniques for Bio-imaging: Advanced Microscopy and Spectroscopy in Life and Environmental Sciences (ICTP - Trieste, Italy) - February 12 -24, 2017 <http://indico.ictp.it/event/7920/>
- Winter School on Quantitative Systems Biology (ICTP - Trieste, Italy) - December 5-16, 2016 <http://indico.ictp.it/event/7661/>
- CASTEP Training Workshop 2013 (Oxford University) - August 19 - 23, 2013 <http://www.castep.org/CASTEP/Workshop2013>
- Advanced School on Scientific Software Development: Concepts and Tools (ICTP - Trieste, Italy) - 20/02/2012 - 2/03/2012 <http://indico.ictp.it/event/a11154/>
- PRACE Winter School, Hybrid Programming on Massively Parallel Architectures (CINECA, Bologna, Italy) - February 6 - 10, 2012 <http://www.cineca.it/page/prace-winter-school>
- ComplexHPC Spring School 2011 (VU University, Amsterdam, The Netherlands) - May 9 - 13, 2011 <http://www.cs.vu.nl/complexhpc2011/>
- Advanced School on High Performance and Grid Computing (ICTP-Trieste, Italy) - May 9 - 13, 2011 <http://indico.ictp.it/event/a10135/>
- 15th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (ICTP - Trieste, Italy) - January 13 - 15, 2011 <http://indico.ictp.it/event/a10124/>
- CETS 2010 - 5th Central European Training School on Neutron Scattering (Budapest, Hungary) - 31/05/2010 - 4/06/2010 <http://www.kfki.hu/~cets>
- School on Synchrotron and Free-Electron-Laser Sources and their Multidisciplinary Applications (ICTP - Trieste, Italy) - 26/04/2010 - 7/05/2010 <http://indico.ictp.it/event/a09142/>
- MolSim 2010: Understanding Molecular Simulation (University of Amsterdam, The Netherlands) - January 4 - 15, 2010 <http://www.cecarn.org/workshop-0-493.html>
- Advanced School in High Performance and GRID Computing - Concepts and Applications (ICTP - Trieste, Italy) - 30/11/2009 - 11/12/2009 <http://hpc-school.escience-lab.org>
- Hands-On Course: KKR Bandstructure and Spectroscopy Calculations (Ludwig-Maximilians-Universität München, Germany) - June 24 - 26, 2009 <http://olymp.cup.uni-muenchen.de/ak/ebert/workshops/2009/KKRHOC2009/>
- Advanced School in High Performance and GRID Computing (ICTP - Trieste, Italy) - November 3 - 14, 2008 <http://indico.ictp.it/event/a07176/>
- First principles molecular dynamics simulations in condensed matter and molecular physics (CECAM-ENS, Lyon, France) - May 13 - 17, 2008 <http://www.atosim.cecarn.org/workshop-1-229.html>
- School on Pulsed Neutrons: Characterization of Materials (ICTP - Trieste) - November 15 - 26, 2007 <http://indico.ictp.it/event/a06221/>
- 13th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (ICTP - Trieste, Italy) - January 11 - 13, 2007 <http://indico.ictp.it/event/a06178/>
- Summer School on Electronic Structure Methods and Their Applications, and Workshop on Computational Materials Theory (Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India) - July 10 - 22, 2006 <http://www.jncasr.ac.in/smr1783/>
- NANOMA 2005 - Physics and Chemistry of Nanomaterials (Babeș-Bolyai University, Cluj-Napoca, Romania) - 21/08/2005 - 03/09/2005 <http://phys.ubbcluj.ro/nanoma/>
- BiImage Summer School 2005 (Ecole Normale Supérieure, Paris, France) - 11/06/2005 - 22/06/2005 <http://www.ecole2005.ibpc.fr>

## Membru al:

- [Asociației pentru Mașini de Calcul](#)
- [Societății Optice Americane](#)
- [Societății Române de Fizică](#)

