

PERSONAL INFORMATION



Călin Gabriel Floare

 National Institute for Research and Development of Isotopic and Molecular Technologies (NIRDIMT), Cluj-Napoca, Romania

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Sex Male | Date of birth 09/02/1973 | Nationality Romanian

WORK EXPERIENCE

10/1997–Present

Scientific Researcher

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

supervised by Dr. Adrian Pamula and Dr. Mircea Bogdan

- Research Assistant in Mass Spectrometry Laboratory
- Research Scientist III in Nuclear Magnetic Resonance Group
- [Business or sector](#) Research

09/2007–07/2008

Teaching Assistant

Biophysics Department of the University of Medicine and Pharmacy “Iuliu Hațieganu” (Cluj-Napoca, Romania)

supervised by Prof. Constantin Mihai Lucaciu

- Tutor/Teaching Assistant
- [Business or sector](#) Academic Teaching

EDUCATION AND TRAINING

06/2014–06/2016

Master in Molecular Biotechnologies

Babes-Bolyai University, Faculty of Biology and Geology (Cluj-Napoca, Romania)

Title of dissertation thesis: *Streptomyces griseolus* recombinant ferredoxin production

supervised by Prof. Iulia Lupan

06/2000 - 11/2005

PhD. in Physics

Joseph Fourier University (Grenoble I, France)

Title of thesis: Dynamics and reactivity in confined environments

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

supervised by Prof. Hans Peter Trommsdorff and Prof. Simion Astilean

10/1997 - 06/1998

Master in Theoretical Physics

Babes-Bolyai University, Faculty of Physics (Cluj-Napoca, Romania)

Title of dissertation thesis: Tight-binding Molecular Dynamics of the fullerene (C₆₀) molecule

supervised by Prof. Titus Adrian Beu

10/1991 - 06/1997

Diploma in Physics

Babes-Bolyai University, Faculty of Physics (Cluj-Napoca, Romania)

Title of diploma thesis: Molecular clusters of SF₆ - Ar

supervised by Prof. Titus Adrian Beu

RESEARCH STAGES

28/06/2011 - 9/07/2011
1/10/2012 - 8/12/2012

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

'Statistical and Biological Physics' group, supervised by Prof. Alessandro Laio

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

▪ within HPC-Europa 2 project - <http://www.hpc-europa.eu/>

July 9 - 28, 2011

CINECA, Bologna, Italy

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

▪ within HPC-Europa 2 project - <http://www.hpc-europa.eu/>

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

Laue-Langevin Institute, Grenoble, France

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

'Computing for Science' group, supervised by Dr. Mark Johnson

▪ Ph.D. Student

PERSONAL SKILLS

Mother tongue(s) Romanian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	B2	B2	B2	B2	B2
Replace with name of language certificate. Enter level if known.					
French	Good	Good	Good	Good	Good
Replace with name of language certificate. Enter level if known.					

[Common European Framework of Reference for Languages](#)

Communication skills

▪ Ability to interact and effectively communicate with people from diverse backgrounds, highlighting teamwork and problem solving.

Organisational / managerial skills

▪ Research grants member and manager, between 2006-2019

Job-related skills

▪ good expertise in Nuclear Magnetic Resonance, UV-vis, Infrared, Raman and Fluorescence spectroscopies, Mass Spectrometry, X-ray and neutron scattering and diffraction, molecular biology and biotechnology methods

▪ good expertise in computational chemistry and biochemistry methods like: ab initio calculations (Gaussian, Hyperchem, CASTEP, Crystal, VASP), molecular dynamics (AMBER, NAMD, GROMACS, VMD), docking (AutoDock, Vina) and bioinformatics (Galaxy)

▪ software development in C, C++, Fortran, Python, TCL, Octave, Matlab, MPI, CUDA

▪ HPC Linux Cluster Administration: Torque, Maui, IBM LSF, GPFS, Ganglia, Nagios

Digital competence

	SELF-ASSESSMENT				
	Information processing	Communication	Content creation	Safety	Problem solving
	Proficient user	Proficient user	Proficient user	Proficient user	Proficient user

Driving licence

B

ADDITIONAL INFORMATION

Publications

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

- A. Pirnau, 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. Pirnau, **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)
- L. Buimaga-larinca, **C.G. Floare**, A. Farcas, S. Porav, L. Janosi, Use of complementary molecular modeling approaches in search of peptides binding to oncogenic Ras, *European Biophysics Journal with Biophysics Letters* 46(1), S398-S398, P-1077 (2017)
- 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 SrTiO₃ Based Oxides for Thermoelectric Applications, *J. Phys. Chem. C* 120(45) 25678-25688 (2016)
- Alexandra Farcaș, Luiza Buimaga-larinca, **C.G. Floare**, L. Janosi, Effect of complex mammalian membrane models with multiple membrane components on Ras protein nanoclustering, *FEBS JOURNAL* 283 SI(1), 235 (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. Pirnau, 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 Furibiprofen 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, ¹H 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, ¹H NMR investigation of self-association of vanillin in aqueous solution, *J. of Phys.: Conf. Series* 182, 012002 (2009)
- Assa Aravindh et al., Si_xC_{1-x}O₂ 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 Babes-Bolyai, Physica*)
- M. Plazanet, **C. Floare**, M. R. Johnson, R. Schweins, H. P. Trommsdorff, Freezing on heating of liquid solutions, *J. Chem. Phys.*, 121(11), 5031 (2004) & ILL Annual Report 2004, 54-55
- M. Johnson, **C. Floare**, H.-P. Trommsdorff, Ab initio modelling of molecular vibrations in hydrogen-bonded solids, *ISIS Rutherford Appleton Laboratory, Oxford, Experimental Report*, RB 12976 (2003)

Presentations

- 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 SrTiO₃ based oxides for thermoelectric applications
- Cyclodextrin inclusion compounds. Investigation of an unusual phase transition, Scuola Internazionale Superiore 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

Projects

As Project Manager

- HPC-Europa2 Project - Molecular dynamics investigation of an inverse freezing counterintuitive phenomenon (2012). This project financed SISSA and CINECA research stages.
- CEEEX ET-58/18.09.2006 - Experimental, ab initio and molecular dynamics investigation of an unusual phase transition, Total project value: 144,000 RON

As Member

- 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 SrTiO₃ 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)

Schools and Workshops

- 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 (Babeş-Bolyai University, Cluj-Napoca, Romania) - 21/08/2005 - 03/09/2005 <http://phys.ubbcluj.ro/nanoma/>
- Biolmage Summer School 2005 (Ecole Normale Supérieure, Paris, France) - 11/06/2005 - 22/06/2005 <http://www.ecole2005.ibpc.fr>

Memberships

- [Association for Computing Machinery](#)
- [European Physics Society](#)
- [Optical Society of America](#)
- [Romanian Physics Society](#)