

Prof. Gérald MONARD

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Age: 46

Citizenship: French

Personal status: Married, 1 child

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Research keywords: Computational and Theoretical Chemistry; Molecular Modeling;
Quantum Chemistry; Molecular Dynamics;
Semiempirical Methods; Linear Scaling Algorithms;
QM/MM Methods; Biomolecules;
Enzymatic Reactivity; Reaction Paths;

Positions:

since 2016 Director of the EXPLOR High Performance Computing Centre of Université de Lorraine

since 2007 Professor of computational chemistry, Université de Lorraine

2012-2016 Project manager for Université de Lorraine in charge of building a new HPC Centre

1999-2007 Associate Professor of computational chemistry, Université Henri Poincaré - Nancy I

1998-1999 Post-doctoral fellow, Pennsylvania State University (group of Prof. Kenneth M. Merz, Jr.)

Education:

2006 Habilitation, Université Henri Poincaré - Nancy I

1994-1998 Ph. D. in Computational and Theoretical Chemistry, Université Henri Poincaré,
under the supervision of Prof. Jean-Louis Rivail

1993-1994 M. S. in Computational and Theoretical Chemistry, University Henri Poincaré - Nancy I

1991-1995 M. S. in Physical Chemistry, Ecole Normale Supérieure de Lyon (ENS Lyon)

1989-1991 "Classes préparatoires aux Grandes Ecoles", Louis-Le-Grand, Paris

Research record

- Scientific production: 44 articles in international peer reviewed journals
- Other publications: 3 book chapters
- h-index factor = 19 (Source: Google Scholar)
- Invited talks in national or international meetings: 19
- Invited talks in institutions: 13

Students supervised: 11 M.S. students, 8 Ph.D. students

Grants, Honors & Awards

- Scientific collaborations (as Principal Investigator):
 - Bogazici University, Turkey (PHC Bosphorus: 2006-07, CNRS-Tubitak: 2009-10 & 2013-14)
 - Istanbul Technical University (PHC Bosphorus: 2014-15, 2016-17)
 - University of Copenhagen (French Embassy: 2010 & French-Danish mobility program: 2010)
- Research contract: Sanofi-Aventis (P.I. 2003-05); Aventis Pharma (P.I. 2001-02)
- As a participant: ACI GRID (GRID-ASP: 2002-05), ACI IMPBio (SIRE: 2004-07), ANR Blanche (CREAM: 2009-12)

Conferences organized or co-organized: 2 CECAM workshops, 1 ACS meeting

Teaching: ~150 hours/year.

All media I used for teaching are publicly available on my web site (<http://www.monard.info>)

- Chemical Bonding (B. Sc. in Physics & Chemistry)
- Chemical Bonding (B. Sc. in Biology)
- Molecular Modeling (M. S. in Chemistry)
- Biochemistry for chemists (M. S. in Chemistry)
- High Performance Computing (M. S. in Chemistry & Doctorale level)
- Computational tools: python, bash scripting, *etc* (M. S. in Chemistry & Doctoral level)

Invited lectures: 7 (Belgium, Luxembourg, CNRS/France)

Academic duties:

- Director of the regional HPC Centre EXPLOR hosted by Université de Lorraine (3.1M € of budget for 2015-18; ~6,000 cores, ~2 Po of storage)
- Elected member of the laboratory council (SRSMC laboratory, 2015-17)
- Board member of the CNRS Research Group CORREL (Correlated Methods for Electronic Structure, 2011-15)
- Board member of the French Network of Theoretical Chemistry (2010-18)
- Creator and maintainer of the nationwide French Network of Theoretical Chemistry mailing-list (rctf-membres@asso.univ-lorraine.fr, since 2006, > 400 subscribers)

Expertise and editorial activities:

- Member of the AMBER software development team
- Expert for Agence Nationale de la Recherche (ANR), French and European Computing Facilities (GENCI & PRACE)
- Board member of the Scientific Council of the HPC centre of the Université de Strasbourg (since 2017)
- Member of Ph.D. thesis committees: 19 included 4 abroad (Spain, Turkey)
- Panel member for academic hiring: 4
- Referee for various peer review journals (in the last five years): *J. Phys. Chem.*, *J. Chem. Theory Comput.*, *J. Molec. Model.*, *Theor. Chem. Acc.*, *J. Mol. Biochem.*, *Eur. J. Med. Chem.*, *J. Chem. Inf. Model.*, ...)

Other skills

- Computer programming: C, Fortran, Python, MPI, OpenMP, High Performance Computing (HPC)
- Use of various HPC national and regional centres; GPU computations
- Web development (html, wiki, SQL, mailing-list)
- Software development: git
- Hardware and Software administration (installation and administration of a local ~500 core cluster): Linux administration, Queueing system (SGE), NFS, Storage arrays, etc.