

Dr Fan WANG, Ph.D.

LG2A, CNRS FRE 3517, UFR de Pharmacie,
Université de Picardie Jules Verne
1, rue des Louvels
80036 Amiens Cedex, France
E-mail: fan.wang@u-picardie.fr
fan.wang@q4md-forcefieldtools.org
Web site: <http://q4md-forcefieldtools.org/FW>
Phone number: +33-6-2853-7733
Citizenship: Chinese
Date of birth: August 1986

Present situation

Research scientist associated to the q4md-forcefieldtools project
Searching for a position in the academic field (in computational Chemistry, bioinformatics or scientific calculation)

Education

- Oct 2014 **Ph.D. in Computational Chemistry**
Title: Software developments and structural studies of bioinorganic complexes by molecular dynamics.
Manuscript: <http://q4md-forcefieldtools.org/FW/Thesis>
- 2010 **MS in Computer Science and Technology**
Université de Picardie Jules Verne, Amiens, France
- 2008 **BS in Computer Science and Technology**
Université de Picardie Jules Verne, Amiens, France
- 2007 **BS in Mathematics**
Université de Picardie Jules Verne, Amiens, France
- 2005 **First year undergraduate in Mathematics**
Huazhong University of Science and Technology, Wuhan, China

Skills and Achievements

Scientific computing and molecular modeling and software:

- Development of the PyRED (or R.E.D. Python, Python programming language) and R.E.D. Server Development tools (<http://q4md-forcefieldtools.org/REDServer-Development>) for force field generation (Amber and Glycam force fields).
- Optimization of the R.E.D. IV program (Perl programming language)
- Molecular dynamics simulation using the pmemd and sander programs (AMBER)
- Visualization (VMD, GaussView, Avogadro, PyMol)
- Quantum chemistry (Gaussian, GAMESS, Firefly)
- Babel (file format conversion), BKchem

Programming and Operating Systems:

- Development with languages : Python, Perl, C/C++, Fortran, Java
- Web development : XHTML, PHP, JavaScript, MySQL, CSS
- Experience with software for mathematics (Matlab, Scilab)
- MPI and OpenMP parallel programming
- Shell scripting (tcsh, bash, sed, awk)
- Installation and management of Linux on workstations and cluster of computers (administration, program installation and compilation, PBS queuing system)

Languages

Chinese	native
French	written, read, spoken
English	written, read, spoken

Research Experience

Oct 2011 - Nov 2014:

LG2A, CNRS FRE 3517, UFR de Pharmacie, Université de Picardie Jules Verne

Ph.D. student, Supervisor: Professor F.-Y. Dupradeau

- **Project: Empirical force field development with an object oriented programming approach and molecular dynamics simulation of bioinorganic complexes**
- **International French-USA project between the Université de Picardie Jules Verne and the Sanford Burnham Medical Research Institute (San Diego, USA)**
- **Scholarship from the "Conseil Régional de Picardie" and the "European Regional Development Fund"**

Jan 2010 - Aug 2010:

Doonya Technologies, Lille, France - Université de Picardie Jules Verne

Master, Supervisor: Professor A. Lapujade

- **Project: Development of the application WebConf for controlling the conference of Voice Over Internet Protocol (VOIP Asterisk, QoS, PHP, Javascript, C/C++, Linux)**

Publications

- *Object oriented programming for Amber force fields: application to the study of bioinorganic complexes by molecular dynamics simulation*
F. Wang, J.-P. Becker, P. Cieplak, F.-Y. Dupradeau, in preparation.
- *β -hematin crystal formation: first insights from molecular dynamics of small clusters in water*
J.-P. Becker, F. Wang, P. Sonnet, F.-Y. Dupradeau, J. Am. Chem. Soc. submitted Jul 28, 2015.

- *Effects of Hypoxanthine Substitution in Peptide Nucleic Acids Targeting KRAS2 Oncogenic mRNA Molecules: Theory and Experiment*
J. M. Sanders, M. E. Wampole, C.-P. Chen, D. Sethi, A. Singh, F.-Y. Dupradeau, F. Wang, B. D. Gray, M. L. Thakur & E. Wickstrom, *J. Phys. Chem. B* **2013**, **117**, 11584-11595.

Communications

- *R.E.D. Python: Application of object oriented programming to charge derivation and force field library building for the Amber additive and non-additive force field models*
F. Wang, J.-P. Becker, P. Cieplak, F.-Y. Dupradeau, GGMM 2013 meeting (Groupe Graphisme et Modélisation Moléculaire), Ile d'Oléron, May 21 – 23, 2013.
- *R.E.D. Python: Object oriented programming for Amber force fields*
F. Wang, J.-P. Becker, P. Cieplak, F.-Y. Dupradeau, 247th American Chemical Society national meeting, Dallas, TX, March 16-20, 2014.

Program, web server and tutorials

- *R.E.D. Server Development - Performing calculations with the PyRED program : Application to charge derivation, force field library building and force field parameter generation*
Fan Wang, [1] Jean-Paul Becker, [1] Piotr Cieplak, [2] François-Yves Dupradeau [1] [1] FRE CNRS 3517 & UFR de Pharmacie, Université de Picardie - Jules Verne, rue des Louvels, Amiens, France
[2] Sanford | Burnham Medical Resesearch Institute, 10901 North Torrey Pines Road, La Jolla, CA 92037, USA
<http://q4md-forcefieldtools.org/Tutorial/Tutorial-4.php>
<http://q4md-forcefieldtools.org/REDServer-Development>

References

- **F.-Y. Dupradeau**, Professor of chemistry; LG2A, CNRS FRE 3517, UFR de pharmacie, Université de Picardie Jules Verne
E-mail: fyd@u-picardie.fr, Phone number: +33-3-2282-7498
- **P. Cieplak**, Research Associate Professor; The Sanford Burnham Medical Research Institute, San Diego, USA
E-mail: pcieplak@sanfordburnham.org, Phone number: +1-858-646-3100 x 3076
- **Y. Li**, Professor of Computer Science and Technology; UFR de Mathématiques et d'Informatique, Université de Picardie Jules Verne
E-mail: yu.li@u-picardie.fr, Phone number: +33-3-2282-7872