

## Wenjin Li

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### Highlights

- Solid background in Molecular Dynamics, especially skilled in QM/MM simulations and method developments
- Extensive experience in : Linux/Unix, C/C++, Perl, shell scripting
- Strong communication skills (oral and written in English); several first-author publications in peer-reviewed journals
- Creative, well-organized, strong problem-solver

### Education

- Since 2007 Combined M.S. and Ph.D. in Computational Biology  
CAS-MPG Partner Institute for Computational Biology, Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai, China. (Advisor: Dr. Frauke Graeter)
- 2000-2004 B.S. in Bioengineering, College of Materials Science and Chemical Engineering  
Zhejiang University (Project 985), Hangzhou, China.

### Research Experience

Nov. 2009-Nov. 2010

#### Visiting Scientist, Heidelberg Institute for Theoretical Studies

- Implemented transition path sampling in Gromacs
- Investigated thiol/disulfide exchange with transition path sampling
- Estimated the rate of thiol/disulfide exchange
- Identified the structures of transition states

Apr. 2010-July 2010

#### Visiting Scientist, Department of Biophysics, Ruhr University Bochum

- Developed multidimensional potential of mean constraint force (MPMCF) method
- Investigated phosphoester hydrolysis in great detail

Nov. 2010-Dec. 2011

#### Visiting Scientist, Max-Planck-Institute for Biophysical Chemistry

- Developed force matching-force distribution analysis (FM-FDA) method
- Decomposed the mechanical effect on a ring opening reaction

### Other Experiences

- Aug. 2004-Nov. 2005 Management Trainee, Ningbo Rayon Acrylic Fibers Co., Ltd.

### Honors and Awards

- 2011 Shanghai Institutes for Biological Sciences Special Award (Top 10 Student)
- 2009-2011 Sino-Euro PhD Joint Training Program. Only outstanding doctoral students in Chinese Academy of Sciences will be selected
- 2009-2010 Excellent Student Award in Shanghai Institutes for Biological Sciences

### Scientific Skills

- Excellent training in Molecular Dynamics Simulations, especially in QM/MM simulations and Quantum Calculations
- Thorough knowledge in free energy calculations and related methods, such as Umbrella Sampling, Metadynamics and MPMCF. And extensive practices in resolving mechanisms of chemical

- reactions with methods such as transition path sampling and conformational flooding
- Mastered Software: Gromacs, Gaussian, MATLAB, PyMOL, VMD, especially in the application and modification of Gromacs
  - Computational skills: Linux/Unix, C/C++, Perl, shell scripting

## Publications

1. **W. Li**, K. Lin, K. Feng, and Y. Cai. "Prediction of protein structural classes using hybrid properties." *Molecular Diversity*, **2008**, 12, 171-179.
2. L. Chen, L. Lu, K. Feng, **W. Li**, J. Song, L. Zheng, Y. Yuan, Z. Zeng, K. Feng, W. Lu, and Y. Cai. "Multiple classifier integration for the prediction of protein structural classes." *Journal of Computational Chemistry*, **2009**, 30, 2248-2254.
3. **W. Li**, and F. Graeter. "Atomistic evidence of how force dynamically regulates thiol/disulfide exchange." *Journal of the American Chemical Society*, **2010**, 132, 16790–16795.
4. **W. Li**, K. Gerwert, T. Rudack, F. Graeter, and J. Schlitter. "New insights into phosphoester hydrolysis from multi-dimensional free energy surfaces." Submitted.
5. **W. Li**, S. Edwards, L. Lu, T. kubar, F. Graeter, and G. Groenhof. "Decompose the mechanical effect on chemical reactions by force distribution analysis in quantum system." In preparation.

## Presentations/Posters

1. Talk: "Evidence of mechanical regulation on thiol/disulfide exchange from TPS and QM/MM study", 24th Molecular Modelling Workshop, Erlangen, Germany, March 15<sup>th</sup>-16<sup>th</sup>, 2010
2. Poster: "Mechanical regulation of disulfide reduction from QMMM transition path sampling", Workshop on Computer Simulation and Theory of Macromolecules, Huenfeld, Germany. April 16<sup>th</sup>-17<sup>th</sup>, 2010.
3. Poster: "Atomistic evidence of how force dynamically regulates thiol/disulfide exchange", Workshop on Multiscale Molecular Modelling, Edinburgh, UK, June 30<sup>th</sup>- July 3<sup>rd</sup>, 2010.
4. Poster: "Towards a method of force distribution analysis in quantum mechanical system", Workshop on Computer Simulation and Theory of Macromolecules, Huenfeld, Germany. April 15<sup>th</sup>-16<sup>th</sup>, 2011.
5. Poster: "New insights into the mechanism of mechanical regulation on thiol/disulfide exchange". The 8<sup>th</sup> European Biophysics Congress, Budapest, Hungary, August 23<sup>rd</sup>-27<sup>th</sup>, 2011.
6. Poster: "Mechanochemistry of small molecules: into which bond does the force go?" Biophysical Society 56th Annual Meeting, San Diego, February 25<sup>th</sup>-29<sup>th</sup>, 2012.

## References

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