

## Zilu Wang

### ADDRESS

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### EDUCATION

- 2013- Postdoc Fellow, in Prof. Elena Dormidontova group, Institute of Material Science, University of Connecticut. Storrs, CT
- 2013 Ph.D. in Material Chemical Engineering, Department of Chemical Engineering, Tianjin University  
Dissertation title: "Study on the phase behavior of a single polymer chain and its transport kinetics in channel".  
(Advisor: Prof. Dr. Xuehao He, Tianjin University, China).
- 2009 M.S. in Material Chemical Engineering, Department of Chemical Engineering, Tianjin University.  
Thesis title: "Force field development and application of coarse-grained molecular dynamics".  
(Advisor: Prof. Dr. Xuehao He, Tianjin University, China).
- 2007 Dual B.S. in Material Chemistry & Computer Science and Technology,  
Department of Material Science and Technology, Department of Computer Science and Technology,  
Tianjin University, China.

### PERSONAL DETAILS

- Citizenship: Chinese, & married to Li Zuo (Chinese citizen).
- Language: Chinese (Native), English (Fluent), German/Japanese (Basic).

### RESEARCH INTERESTS

Briefly, my primary research goal is to obtain a deeper understanding about the properties of the soft matter system using molecular simulation techniques, particularly in (1) the thermodynamic transition & the kinetic behavior of polymer system with complex topology or sequences. (2) the self-assembly mechanisms of the amphiphilic molecules especially on the self-assembly pathway and the formation of metastable structure. Meanwhile, developing new simulation model and algorithm is another important part in my research in order to dig out more undiscovered mechanism in molecular biology, biophysics and material science. My research interests are mainly as follows:

- Employing coarse-grained molecular dynamics simulation techniques, such as the Iterative Boltzmann Inversion, Force Matching and Multi-Scale Coarse Graining algorithm, or using predefined CG force field to reduce the large degree of freedom in complex system, including force fields design and parameterizing.
- Developing novel Accelerated Sampling Techniques to explore the thermodynamic properties of nonlinear polymer architectures and bio-macromolecules.
- Transport kinetics of macromolecules in ratchet system beyond equilibrium state.
- Large scale nano-fluidic system simulation accelerated by Graphic Processing Unit (GPU).
- Developing novel molecular simulation method and novel types of force field such as the reactive, polarized and anisotropic force field.
- Exploring hybrid/coupling simulation method with the existing methods to obtain a better description.

- Meso-scale simulation of amphiphilic copolymer self-assembly using polymer self-consistent field theory (SCFT).

## TECHNICAL BACKGROUND

- Proficient in CPU & GPU parallel programming techniques using CPU programming language (C/C++, Fortran with OPENMP or MPI interface) and GPU programming language (CUDA). Scripting languages for data process (tcl/tk, Python, Shell) under Linux environment are daily used. Preparing manuscript with Word and Latex.
- Building up and maintenance of Linux cluster and personal super computer.
- Hacking level understanding of GROMACS and HOOMD package both in software architectures and algorithms. Familiar with NAMD, ESPResSo, DPDmacs and Gaussian 09 and some data visualizing software such as VMD, Origin, Matlab, OpenDX and OpenGL interfaces.
- In house software development:
  - **MagicMD**: a coarse-grained molecular dynamic package running on GPU, suitable for simulating large-scale molecular system. (Developers: Zilu Wang, Zhe Jia, Rui Xu)
  - **WLD-BFM**: a package for calculating thermodynamic transition of polymer system, using refined parallel Wang-Landau sampling algorithm. (Developers: Zilu Wang, Long Wang)
  - **SCFT-GPU**: a GPU based software package for simulating self-assembly of blocked copolymer in solution employing polymer self-consistent field theory. (Developers: Zilu Wang)

## HONOR AND AWARDS

- Shanghai Pudong Development Bank Scholarship, 2011.
- NVIDIA™ CUDA™ Programming Contest 3<sup>rd</sup> prize, China, 2010.
- Outstanding doctoral thesis fund, 2009.

## HOBBY

Reading, Swimming, Ping Pong & Making demo scene (computer art).

## PUBLICATIONS

### Journal Articles:

#### -2014-

**Zilu Wang**, Long Wang, Yu Chen, Xuehao He\* (2014): Phase transition behaviours of a single dendritic polymer. *Soft Matter* 10 (23), 4142-4150

Huaping Li, **Zilu Wang**, Ningning Li, Xuehao He\* and Haojun Liang (2014): Denaturation and renaturation behaviors of short DNA in a confined space. *J. Chem. Phys.*, 141, 044911.

#### -2013-

**Zilu Wang**, Zhe Jia, and Xuehao He\* (2013): Net motion of a charged macromolecule in a ratchet-slit. *Soft Matter*. 2013, 9, 11107-1112.

**Zilu Wang**, Long Wang, and Xuehao He\* (2013): Phase Transition of a Single Protein-like Copolymer Chain. *Soft Matter*. 2013, 9 (11), 3106 – 3116.

Rui Xu, **Zilu Wang**, Xuehao He\* (2013): Dynamics of Vesicle Formation from Lipid Droplets II: Influences of HPC and DPPC composition ratio. *Chin. J. Chem. Phys.* 26(2), 203.

**-2012-**

Long Wang, Rui Xu, **Zilu Wang** and Xuehao He\* (2012): Kinetics of multicompartement micelle formation by self-assembly of ABC miktoarm star terpolymer in dilute solution, *Soft Matter* 8, 11462-11470.

**-2011-**

**Zilu Wang** and Xuehao He\* (2011): Phase Transition of a Single Star Polymer: a Wang-Landau Sampling Study. *J. Chem. Phys.* 135, 094902(1-10).

**-2009-**

**Zilu Wang** and Xuehao He\* (2009): Dynamics of Vesicle Formation from Lipid Droplets: Mechanism and Controllability. *J. Chem. Phys.* 130, 094905(1-8).

**Contributions to Academic Conferences**

Bo Du, **Zilu Wang** and Xuehao He\*. (2012) Developing coarse-grained force fields of poly(methylmethacrylate-b-2-vinylpyridine) from atomistic simulation. ICMEAC Conference, also in *Advanced Materials Research* Vols. 562-564 pp 123-128.

Bo Du, **Zilu Wang** and Xuehao He\*. (2011) Computer simulation of self-assembly of dumbbell-shaped supramolecules. International Conference on Nanoscience & Technology.

**Zilu Wang** and Xuehao He\* (2010) Thermodynamic behavior of single star polymer chain: Wang-Landau sampling. 27<sup>th</sup> CCS Congress (Xiamen, China).

**Zilu Wang** and Xuehao He\* (2009) Developing coarse-grained force fields for PNIPAM single chain from the atomistic model. ICBBE 3<sup>rd</sup> International Conference (Beijing, China).

**Zilu Wang** and Xuehao He\* (2008) Vesicle formation from lipid small ball in water: a molecular dynamics investigation. 26<sup>th</sup> CCS Congress (Tianjin, China).