

# Minye Zhang

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## EDUCATION

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- **Peking University - Beijing, P.R.China**  
- B. Sc in chemistry **GPA: 3.40/4.00** Sept. 2011 – Jul. 2014  
College of Chemistry and Molecular Engineering
- **Uppsala University - Uppsala, Sweden**  
- Exchange student Jan. 2014 - Jun. 2014  
Department of Chemistry – BMC
- **Computer Skills:** Languages: C, Fortran, Bash Shell. Softwares: Amber, AutoCAD,, Chemoffice, Endnote, Gaussian, Origin.

## ACADEMIC EXPERIENCES

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- **Computational Study on Cross-hyperconjugated Compounds**  
Department of Chemistry – BMC, Uppsala University Mar. 2014 – Jun. 2014  
Supervisor: Prof. Henrik Ottosson  
-Objectives: to pinpoint compounds with good optical properties from a class of polycyclic molecules featuring cross-hyperconjugation with a group 14 element four-membered ring, the strategy of synthesis.  
-Responsibilities: geometry optimization and excited state calculation by DFT and TD-DFT methods to obtain optical properties, ring strain study with homodesmotic reaction and group equivalent methods, examination on the origin of the strain.
- ***Ab Initio* Molecular Dynamics Simulations of Vibrational Spectra of trans-Stilbene (Dissertation Work)**  
College of Chemistry and Molecular Engineering, Peking University Mar. 2015 – Jun. 2015  
Supervisor: Prof. Jian Liu  
-Objectives: to simulate the IR and Raman spectra of trans-Stilbene by *ab initio* molecular dynamics (AIMD) and compare them with the experimental results; to verify the necessity of quantum dynamic method in generating the density of configurations by comparing structural parameters obtained with classical MD and path integral molecular dynamics (PIMD).  
-Responsibilities: to perform AIMD by Amber and Gaussian; to compose the codes of auto correlation functions of dipole and polarizability and code of Fourier transformation; to write shell codes for batch process.

## SOCIAL PRACTICES

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- Co-author of a Chinese science fiction, *Republic of Molecules* Apr. 2013
- Group leader of volunteers in Youth Camp of All-China Federation of Taiwan Compatriots Jul. 2012, Jul. 2013
- Volunteer in 29<sup>th</sup> Chinese Chemical Society Congress Aug. 2014

- The Secretary-General of College Student Union Sept. 2012 – Jun. 2013
- Director of the Department of the Students' Rights of College Student Union Sept. 2012 – Jun. 2013

## **HONORS**

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- First Prize in Chemistry Olympic Competition (provincial level) Nov. 2010
- Granghua Scholarship, Peking University May. 2012
- Merit Student, Peking University Mar. 2012, Mar. 2013
- Education Abroad Program Scholarship, Peking University Nov. 2014

## **HOBBIES**

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Basketball, baseball, RPG games, Anime