

CURRICULUM VITAE

Yinghua Shen

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EDUCATION

Ph.D. in Physical Chemistry **Dartmouth College** 09/2000-09/2005
Advisor: Prof. Joseph J. BelBruno

Bachelor of Science in Chemistry **Xiamen University (P.R. China)** 09/1993-07/1997

TEACHING EXPERIENCE

Teaching Assistant Department of Chemistry, Dartmouth College 09/2000-06/2003
Supervising six terms of undergraduate physical chemistry lab, responsibilities include: presenting laboratory lectures, setting up instructional lab experiments, demonstrating usage of lab instruments, grading the reports, answering the students' questions related to the labs outside labs.

Teaching Assistant Department of Chemistry, University of Alberta (Canada) 09/1999-04/2000
Supervising two terms of undergraduate general chemistry labs. Presented laboratory lectures, demonstrated usage of lab instruments, graded lab reports and exams, answered the students' questions related to the labs.

RESEARCH EXPERIENCE

Ph.D. Thesis 09/2000-present
Dissertation title: "Computational studies of small IB clusters and their van der Waals complexes"
Exploration of the properties of small IB clusters using ab initio methods (Density Functional Theory and Coupled-Cluster method), with special focus on: (1) The interaction of small IB clusters with a graphite surface, looking into their surface adsorption energies and electronic structures; (2) The Jahn-Teller effect of the trimers and their Van der Waals molecules, calculation of their Born-Oppenheimer hypersurfaces for the explanation of the experimental spectroscopic results and prediction of their vibronic energy level and vibrational-rotational energy levels.

B.A. Thesis 03/1997-07/1997
Thesis: "Synthesis of carbon nanotube by way of catalytic decomposition of CH₄"
Developed synthetic methodology of carbon nanotubes, characterization of carbon nanotubes produced by catalytic decomposition of CH₄ by different catalysts, and optimization of catalyst synthesis conditions.

NMR lab, Xiamen University (P.R. China) 12/1997-08/1998

Study of catalysts by ^{51}V NMR. Investigated the possibility of using solid state NMR to follow catalysis process *in situ*.

Computational Chemistry Center, Xiamen University (P.R. China)

11/1998-02/1999

Ab initio calculation of NMR parameters of Group VIII metal catalysts

HONORS AND AWARDS

Graduate School

John H. Wolfenden Teaching Prize	09/2003
Awarded to graduate students in chemistry who have demonstrated outstanding performance in teaching.	
Dartmouth Filene Teaching Award	06/2004
Awarded to graduate students in Dartmouth College who have demonstrated outstanding performance in teaching.	
Arts and Sciences graduate fellowships	09/2000
Excellent Teaching Assistant award (University of Alberta, Canada)	03/2000

Undergraduate School

Excellent Student award	1998
First Prize of Ruian Scholarships for overall undergraduate study	1997
Excellent Student award for 3 consecutive years	1994 to 1997
Academic Excellent Scholarships for 4 consecutive years	1993 to 1997

PUBLICATIONS

Journal Articles

- Y. Shen**, J. J. Belbruno, "DFT study of interaction between small IB clusters and a graphite surface", (in preparation).
- Y. Shen**, J. J. Belbruno, "Density functional theory study of ground and excited states of neutral and ionic CuAr and CuKr van der Waals complexes", *J. Phys. Chem. A*. (in preparation).
- Y. Shen**, J. J. Belbruno, "TDDFT study of the excited states of Cu_3Ar and Cu_3Kr : Blue shifts in the photodissociation spectra", *J. Chem. Phys.* (submitted).
- Y. Shen**, J. J. Belbruno, "Ground state potential energy surfaces for Cu_3Ar and Cu_3Kr ", *J. Chem. Phys.* (submitted).
- Y. Shen**, J. J. Belbruno, "An EOM-CCSD study of the excited states of CuAr and CuKr", *J. Phys. Chem. A*. (submitted)
- Y. Shen**, J. J. Belbruno, "Studies of neutral and ionic CuAr and CuKr van der Waals complexes", *J. Phys. Chem. A* (in press)
- Y. Shen**, J. J. Belbruno, "A density functional theory study of the Jahn-Teller effect and spin-orbit coupling for copper and gold trimers", *J. Phys. Chem. A*, 109, 512 (2005).
- Y. Shen**, J. J. Belbruno, "Ag₃ Born-Oppenheimer potential hypersurfaces", *J. Chem. Phys.*, 118, 9241 (2003).