

# CURRICULUM VITAE

## Dr. Hee-Seung Lee

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U. of North Carolina Wilmington  
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### Education:

- June 1996 - December 2001 : Ohio State University  
Ph.D. in Theoretical Chemistry  
Thesis title: Structure, spectroscopy and dynamics of small van der Waals complexes
- 1994 - 1996 : Seoul National University (Korea)  
M.S. in Physical Chemistry  
Thesis title: Excitation mechanism in the collision-induced dissociation  
of methane molecular ion at keV translational energy
- 1988 - 1992 : Seoul National University (Korea)  
B.S. in Chemistry

### Professional Experience:

- February 2004 - July 2007 : New York University  
Postdoctoral Research Associate
- January 2002 - January 2004 : University of Chicago  
Postdoctoral Research Associate

### Honors:

- Presidential Fellowship, Ohio State University, 2001
- McPherson Fellowship, Ohio State University, 2000
- Presidential Fellowship, Seoul National University, 1990 - 1991

### Teaching Experience:

- 1997-1998: Teaching assistant, Ohio State University  
General Chemistry (Laboratory) and Physical Chemistry (Recitation)
- 1995-1996: Teaching assistant, Seoul National University  
General Chemistry (Laboratory)
- Fall 2007: General Chemistry (Lecture)

## Affiliation:

- Americal Chemical Society

## Research Interest:

- Oxidation/Reduction reactions on the fuel cell electrodes with carbon nanotubes:
  - *Ab initio* simulations of metal doping on carbon nanotubes
  - Investigating the role of metal doped carbon nanotubes on the oxidation and reduction reactions on electrodes
- Organic functionalization of semiconductor surfaces :
  - Identifying the mechanism and reaction intermediates involved in reactions between unsaturated hydrocarbons and semiconductor surfaces
- Metal ion complexes in biological systems :
  - Investigating the nature of interactions between the metal ion complexes and DNA or proteins
- Dynamics in condensed phase media:
  - *Ab initio* simulations of solvation structure and ion transport mechanism in highly concentrated acidic and basic solutions
- Developing new *ab initio* MD simulation techniques :
  - Car-Parrinello *ab initio* MD using localized real-space basis
  - Linear scaling *ab initio* MD based on orbital localization scheme
- Density functional theory :
  - Efficient implementation of hybrid functionals for the *ab initio* MD using localized real-space basis.
- Parallel implementation of large scale molecular dynamics code
  - Currently, a member of PINY\_MD and OPEN\_ATOM parallel code development team

## Recent Presentations:

1. “*Ab initio* molecular dynamics studies of proton transport mechanisms in the superprotonic phase of  $\text{CsH}_2\text{PO}_4$ ”  
232<sup>th</sup> ACS national meeting (September 2006, San Francisco)
2. “Combined *ab initio* and extended valence bond molecular dynamics studies of liquid/vapor interface of HCl solution”  
230<sup>th</sup> ACS national meeting (August 2005, Washington D.C.)
3. “Efficient evaluation of nonlocal pseudopotentials via Euler exponential spline”  
ACS 37<sup>th</sup> Midatlantic regional meeting (May 2005, New Brunswick, NJ)

## List of publications:

20. **Hee-Seung Lee** and Mark E. Tuckerman  
“Dynamical properties of liquid water from *ab initio* molecular dynamics in the complete basis set limit” *J. Chem. Phys.* **126** 164501 (2007)
19. **Hee-Seung Lee** and Mark E. Tuckerman  
“Structure of liquid water at ambient temperature from *ab initio* molecular dynamics in the complete basis set limit” *J. Chem. Phys.* **125** 154507 (2006)
18. **Hee-Seung Lee** and Mark E. Tuckerman  
“*Ab initio* molecular dynamics simulation with discrete variable representation basis sets: Techniques and application to liquid water” *J. Phys. Chem. A* **110** 5549 (2006)
17. **Hee-Seung Lee**, Mark E. Tuckerman and Glenn J. Martyna  
“Efficient evaluation of nonlocal pseudopotentials via Euler exponential spline interpolation” *ChemPhysChem* **6** 1827 (2005)
16. **Hee-Seung Lee** and John C. Light  
“Vibrational energy levels of ozone up to dissociation revisited”  
*J. Chem. Phys.* **120** 5859 (2004)
15. **Hee-Seung Lee** and John C. Light  
“Iterative solutions with energy selected bases for the highly excited vibrations of tetra-atomic molecules”  
*J. Chem. Phys.* **120** 4626 (2004)
14. **Hee-Seung Lee**, Hua Chen and John C. Light  
“Symmetry-adapted direct product discrete variable representation for the coupled angular momentum operator: Application to the vibrations of  $(\text{CO}_2)_2$ ”  
*J. Chem. Phys.* **119** 4187 (2003)
13. **Hee-Seung Lee** and John C. Light  
“Molecular vibrations: Iterative solution with energy selected bases”  
*J. Chem. Phys.* **118** 3458 (2003)
12. **Hee-Seung Lee** and Anne B. McCoy  
“Theoretical studies of the vibrational states of  $\text{Ne}_2\text{SH}$  and  $\text{Ne}_2\text{OH}$  ( $A^2\Sigma^+$ )”  
*J. Chem. Phys.* **116** 9677 (2002)
11. **Hee-Seung Lee** and Anne B. McCoy  
“Theoretical studies of rotational and spin-orbit predissociation of the  $\text{NeXH}$  ( $X^2\Pi$ ,  $X=\text{O},\text{S}$ ) van der Waals complexes”  
*Phys. Chem. Chem. Phys.* **4** 1564 (2002)

10. **Hee-Seung Lee** and Anne B. McCoy  
 “Quantum Monte Carlo studies on the structure and spectroscopy of the  $\text{Ne}_n\text{OH}$  ( $A^2\Sigma^+$ ,  $n = 1 - 4$ ) van der Waals complexes”  
*J. Chem. Phys.* **114** 10278 (2001)
9. Slawomir. M. Cybulski, Rafal. R. Toczyłowski, **Hee-Seung Lee** and Anne. B. McCoy  
 “Theoretical studies of the  $\tilde{X}^2\Pi$  and  $\tilde{A}^2\Sigma^+$  states of the  $\text{Ne}\cdot\text{SH}$  and  $\text{He}\cdot\text{SH}$  complexes”  
*J. Chem. Phys.* **113** 9549 (2000)
8. **Hee-Seung Lee**, Anne. B. McCoy, Rafal. R. Toczyłowski and Slawomir. M. Cybulski  
 “Theoretical studies of the  $\tilde{X}^2\Pi$  and  $\tilde{A}^2\Sigma^+$  states of the  $\text{Ne}\cdot\text{OH}$  and  $\text{He}\cdot\text{OH}$  complexes”  
*J. Chem. Phys.* **113** 5736 (2000)
7. Christopher C. Carter, **Hee-Seung Lee**, Anne B. McCoy and Terry A. Miller  
 “The structure of floppy molecules: the  $\text{Rg}\cdot\text{XH}/\text{D}$  ( $\text{Rg}=\text{Ar},\text{Ne}$  and  $\text{Kr}$ ,  $\text{X}=\text{O}$  or  $\text{S}$ ) family of complexes” (review article)  
*J. Mol. Struct.* **525** 1 (2000)
6. **Hee-Seung Lee**, Anne B. McCoy, Larry B. Harding, Christopher C. Carter and Terry A. Miller, “An empirical potential energy surface for  $\text{Ne}\cdot\text{OH}/\text{D}$  complexes”  
*J. Chem. Phys.* **111** 10053 (1999)
5. **Hee-Seung Lee**, John M. Herbert and Anne B. McCoy  
 “Structure and spectroscopy of  $\text{Ne}_n\text{SH}(\tilde{A}^2\Sigma^+)$  complexes using adiabatic diffusion Monte Carlo (ADMC)”  
*J. Chem. Phys.* **111** 9203 (1999)
4. **Hee-Seung Lee**, John M. Herbert and Anne B. McCoy  
 “Adiabatic diffusion Monte Carlo approach for studies of ground and excited states properties of van der Waals complexes”  
*J. Chem. Phys.* **110** 5481 (1999)
3. Christopher C. Carter, Terry A. Miller, **Hee-Seung Lee**, Anne B. McCoy and Edward F. Hayes, “High resolution electronic spectroscopy and an empirical potential energy surface for  $\text{Ne}\cdot\text{SH}/\text{D}$ ”  
*J. Chem. Phys.* **110** 5065 (1999)
2. Christopher C. Carter, Terry A. Miller, **Hee-Seung Lee**, Prakashan P. Korambath, Anne B. McCoy and Edward F. Hayes “High resolution electronic spectroscopy for  $\text{Kr}\cdot\text{OH}/\text{D}$  and an empirical potential energy surface”  
*J. Chem. Phys.* **110** 5065 (1999)
1. **Hee-Seung Lee** and Myung Soo Kim  
 “Excitation mechanism in the collision-induced dissociation of methane molecular ion at kiloelectronvolt translational energy”  
*J. Phys. Chem.* **100** 1459 (1996)

## Book Chapters:

2. John C. Light and Hee-Seung Lee  
“Molecular dynamics: energy selected bases” in *Theory of Chemical Reaction Dynamics (NATO Science Series II)*. Ed. A. Lagana and G. Lendvay, Kluwer (2004)
  
1. Anne. B. McCoy and Hee-Seung Lee  
“Studies of large amplitude motions in weakly bound complexes using diffusion Monte Carlo ”  
in *Wide-Amplitude Rovibrational Bound Bound states in Polyatomic Molecules*  
Ed. M. M. Law, J. Connor and I. Kozin, CCP6 (2002)