

Curriculum Vitae

Shubin Liu

PRESENT POSITION AND ADDRESS:

Senior Computational Scientist
Research Computing Center &
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RESEARCH INTERESTS

Theoretical, conceptual, and computational developments of density functional theory (DFT) and density functional reactivity theory (DFRT) and their applications in biological and material science systems; molecular dynamics modeling and *ab initio* molecular dynamics; quantitative structure-reactivity relationship and applications.

EDUCATION

Jan., 1994 - Sept., 1996: **Ph.D.** Dept. of Chemistry, University of North Carolina,
Major: Physical Chemistry. Advisor: *Robert G. Parr*

Sept., 1985 - June, 1988: **M.S.**, Dept. of Chemistry, Lanzhou University, China
Major: Physical Chemistry. Advisor: *Zhouren Peng*

Sept., 1981 - July, 1985: **B.S.**, Dept. of Chemistry, Hunan Normal University, China
Major: Chemistry

EMPLOYMENT

July 2005 – present Senior Computational Scientist
Research Computing Center
211 Manning Drive, CB# 3420
University of North Carolina at Chapel Hill
Chapel Hill, NC 27599-3420, USA

Sept. 2000 – June 2005 Computational Scientist
Division of Research Computing
Information Technology Services
University of North Carolina at Chapel Hill
Chapel Hill, NC 27599-3455, USA

Oct. 1998 – Aug. 2000 Research Associate (Postdoctoral with *Weitao Yang*)
Department of Chemistry, Duke University
Durham, North Carolina 27708-0359, USA

Oct. 1996 -- Sept. 1998 Research Associate (Postdoctoral with *R.G. Parr* and *Jan Hermans*)
Department of Biochemistry and Biophysics
Department of Chemistry
University of North Carolina at Chapel Hill
Chapel Hill, North Carolina 27599-3290, USA

Jan. 1994 -- Sept. 1996 Research Assistant (Advisor: *Robert G. Parr*)
Department of Chemistry
University of North Carolina at Chapel Hill
Chapel Hill, North Carolina, 27599-3290, USA

July 1988 -- Nov. 1993 Assistant Professor / Lecturer

Department of Chemistry
Hunan Normal University, Changsha, Hunan, China

RESEARCH

- Sept. 2000 – present DFT computational, theoretical and conceptual development and applications in biological and material science related systems; QSAR; Bioinformatics, and linear scaling methods of DFT.
- Oct. 1998 – Aug. 2000 Linear Scaling methods and implementation in DFT; Applications of DFT methods to biological systems.
- Oct. 1996 -- Sept. 1998 Density Functional Theory and its applications; Theoretical study of DNA repairing mechanism and CDA catalysis; Quantum Monte Carlo methods; Mechanism study of photochemical reactions in Environmental Chemistry.
- Jan. 1994 -- Sept. 1996 Density Functional Theory and its applications; Quantum Monte Carlo methods and applications.
- July 1988 -- Aug. 1993 Interpretation of Hund's rule; Force method in Quantum Chemistry; Fermi correlation and Fermi hole; Carbon clusters (Fullerene); Computational Quantum Chemistry.
- Sept. 1985 -- June 1988 Computational Quantum Chemistry (ab initio and semiempirical); Force concept in Chemistry.

COURSES/WORKSHOPS OFFERED

Chem 752, Special Topics in Inorganic Chemistry, Spring 2009 (with Cindy Schauer)
Scientific Computing, UNC-CH, 2005-2010
Shell Scripting, UNC-CH, 2008-2010
Python: An Introduction, UNC-CH 2009-2010
Gaussian/Gaussview, UNC-CH, 2005-2010
Introduction to Computational Chemistry, UNC-CH, 2003-2010
Advanced Computational Chemistry, HNU, 2004-2010
Quantum Chemistry, HNU, 1991-1993
Structural Chemistry, HNU, 1989-1993
Physical Chemistry, HNU, 1992, 1993; *PChem Labs*, HNU, 1988-1993

TECHNICAL SKILLS

Scientific:

Mathematical/Statistical: Maple, Mathematica, Matlab, SAS, SPLUS, Stata, R
Material Science: Cerius2/MS/DS, VASP, ADF/BAND, Felix, CPMD, Crystal
Computational Chemistry: Gaussian, NWChem, GAMESS, Jaguar, ADF, Molpro, ORCA
Computational Biology: SYBYL, InsightII, AMBER, CHARMM, GROMAS, NAMD
Chemo and Bio Database: Cambridge, PDB, NCBI, ASTRAL, MIPS, ExPASy
Chemo and Bio Informatics: ConQuest, BLAST, DSSP, DS Gene, Modeller
Visualization: AVS/Express, Grace/xmgr, ECCE, GaussView, RasMol, Molden, VMD

Computing:

Operation System: UNIX(AIX, IRIX, SOLARIS), LINUX, MacOSX, Windows
Parallel Computing: MPI/MPI2 (MPICH/LAM/MVAPICH/OpenMPI), OpenMP, PVM
Networking: Fast/Gigabit Ethernt, Myrinet, InfiniBand,
Benchmarking: Performance of CPU, Memory, I/O, Compiler/Appls, TOP500.
Languages: FORTRAN 77/90/95, C/ksh Shell Script, HTML/XML, C/C++, Perl, Python

REVIEW SERVICE TO PROFESSIONAL JOURNALS

Journal of the American Chemical Society
Accounts of Chemical Research
Journal of Chemical Physics
Chemical Physics Letters
Physical Chemistry Chemical Physics
International Journal of Quantum Chemistry
Journal of Chemical Theory and Computation
Journal of Theoretical and Computational Chemistry
Journal of Molecular Graphics and Modelling
Reviews of Modern Physics
European Journal of Medicinal Chemistry
QSAR & Combinatorial Science
Australia Journal of Chemistry
Chinese Journal of Chemical Physics
Applied Biochemistry and Biotechnology
Physical Letters A
Food Chemistry
Internt Journal of Science – Biological Chemistry
Letters in Organic Chemistry
Biopolymers
Journal of Photochemistry and Photobiology
Physica A
Journal of Hunan Normal University
Computational and Theoretical Chemistry

Physical Review Letters
Physical Review A-B
Journal of Physical Chemistry A,B,C
Journal of Computational Chemistry
Journal of Physical Organic Chemistry
THEOCHEM
Inorganic Chemistry
Journal of Organic Chemistry
Journal of Molecular Structure
Journal of Cluster Science
Bioorganic & Medicinal Chemistry
Chemical Research in Toxicology
Molecular Diversity
Chemical Physics
New Journal of Chemistry
Journal of Chemical Sciences
Acta Physico-Chimica Sinica
Croatica Chemica Acta
India Journal of Chemistry
Crystal Growth & Design
Structure Chemistry (Chinese)
Chemistry – A European Journal
Progress in Theor. Chem. & Physics

EXTERNAL READER/EXAMINER/REVIEWER

National Science Foundation, USA
Chilean Research Council (FONDECYT), Santiago, Chile
India Institute of Technology, Kharagpur, India
City Universtiy of Hong Kong, Hong Kong, China

ADMINISTRATIVE ACTIVITIES

ITS Topsail Allocation Committee, 2006 – present, ITS, UNC-CH
ITS Exemplar Award Committee, 2005-present, ITS, UNC-CH
IT Awards Committee, 2005-2006, 2010-2011 UNC-CH
Session Chair, 40th IUPAC Congress, Session 4, August 17, 2005, Beijing, China
Session Chair, the 231st ACS Symposium, March 26-30, 2006, Atlanta, GA, USA
Session Chair, 2007 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry. Qingdao, China, August 10-12

PAST & PRESENT COLLABORATORS

North America:

Paul W. Ayers Department of Chemistry, McMaster University, Canada
Lee Bartolotti Department of Chemistry, East Carolina University, USA
Reberto L. Boada Centro de Química, Instituto Venezolano de Investigaciones, Venezuela
N.V. Dokholyan Department of Biochemistry and Biophysics, University of North Carolina, USA
Niri Govind Environmental Molecular Sciences Lab at Pacific Northwest National Lab, USA
Jan Hermans Department of Biochemistry & Biophysics, UNC-CH, USA
Harvey Jeffries Department of Environmental Science & Engineering, UNC-CH, USA

Tonglei Li	Department of Pharmaceutical Sciences, University of Kentucky, USA
Laura E. McNeil	Department of Physics, University of North Carolina, USA
Jim Morken	Department of Chemistry, Boston College, Boston, USA
Robert C. Morrison	Department of Chemistry, East Carolina University, USA
Robert G. Parr	Department of Chemistry, University of North Carolina, USA
Lee G. Pedersen	Department of Chemistry, University of North Carolina, USA
Lalith Perera	National Institute of Environmental Health Sciences , NIH, USA
Cindy K. Schauer	Department of Chemistry, University of North Carolina, USA
Alex Tropsha	School of Pharmacy, University of North Carolina, USA
Alex Y. Wang:	Department of Chemistry, University of British Columbia, Canada
Yue Wu	Department of Physics, University of North Carolina, USA
Weitao Yang:	Department of Chemistry, Duke University, USA
Wei You	Department of Chemistry, University of North Carolina, USA

Europe:

Roberto Cammi	Dipartimento di Chimica Generale, Universita' di Parma, Italy
Frank De Proft	Eenheid Algemene Chemie, Vrije Universiteit Brussel, Belgium
Piotr I. Dem'yanov	Department, Moscow State University, Russia
Paul Geerlings	Eenheid Algemene Chemie, Vrije Universiteit Brussel, Belgium
Paul F. Heelis	Faculty of Science, North East Wales Institute, Deeside, UK
Wilfried Langenaeker	Eenheid Algemene Chemie, Vrije Universiteit Brussel, Belgium
Agnes Nagy	Institute of Theoretical Physics, Kossuth Lajos University, Hungary
JM. Perez-Jorda	Departamento de Quimica Fisica, Universidad de Alicante, Spain
Jean-Philip Piquemal	Laboratoire de Chimie Théorique, Université Pierre Marie Curie, France
M. Torrent-Sucarrat	Eenheid Algemene Chemie, Vrije Universiteit Brussel, Belgium
David J. Tozer	Department of Chemistry, University of Durham, UK
Vladimir Tsirelson	Quantum Chemistry Department, Mendeleev Univ. of Chem. Tech., Russia
Laszlo von Szentpaly	Institut fur Theoretische Chemie, Universitat Stuttgart, Stuttgart, Germany

Asia:

Pratim K. Chattaraji	Department of Chemistry, India Institute of Technology, India
GuanHua Chen	Department of Chemistry, University of Hong Kong, China
Hao Hu	Department of Chemistry, University of Hong Kong, China
Weihai Fang	Department of Chemistry, Beijing Normal University, China
Swapan K. Ghosh	Heavy Water Division, Bhabha Atomic Research Centre, India
Huang Hongxin	Department of Chemistry, Hunan Normal University, China
Samantha Jenkins	Department of Chemistry, Hunan Normal University, China
Ming Lei	Department of Chemistry, Beijing University of Chemical Technology, China
Ji-Chang Xiao	Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, China
Zhong Z. Yang	Department of Chemistry, Liaoning Normal University, China
Dulin Yin	Department of Chemistry, Hunan Normal University, China
Jianguo Yu	Department of Chemistry, Beijing Normal University, China
Zeng Yue	Department of Chemistry, Hunan Normal University, China
Liangren Zhang	School of Pharmaceutical Sciences, Peking University, China
Ruiqin Zhang	Department of Physics, City University of Hong Kong, China
Aiguo Zhong	Department of Chemistry, Taizhou College, Zhejiang, China

HONORS AND AWARDS

1. “*The Information Technology Award*” (team award), University of North Carolina, April 2010.

2. "The Wiley – International Journal of Quantum Chemistry Young Investigator Award", the 46th Sanibel Symposium, St. Simons Island, Georgia, March, 2006.
3. "The Information Technology Award" (individual award), University of North Carolina, April 2005.
4. "Quantum Theory Project (QTP) Stipend Winner", The 40th Sanibel Symposium, University of Florida, Gainesville, Florida, February 2000.
5. "Excellence in Scientific Research and Teaching in the State University System of Hunan Province", Education Committee of Hunan Province, Hunan, Oct., 1993.
6. "Outstanding Faculty in Scientific Research and Teaching", Hunan Normal University, December 1993.
7. "Outstanding Individual in Teaching and Scientific Research in the 1991-1992 Academic Year", Hunan Normal University, December 1992.
8. "Outstanding Achievements in Scientific Research for Junior Faculty", Hunan Normal University, September 1992.
9. "Outstanding General Supervisor", Hunan Normal University, December, 1991.
10. "Outstanding Graduate Student Award", Lanzhou University, Sept., 1987; Sept. 1986
11. "Senior with Highest Honor" (1%), Hunan Normal University, Dec., 1984.
12. "Honored Undergraduate" (8%), Hunan Normal University, Sept., 1983; 1982.

PUBLICATIONS

1. Zhouren Peng, Yizhi Li, and **Shubin Liu**, "On the new method of the semiempirical molecular orbital SCF iteration convergence: inductive diagonal perturbation convergence", *Chinese J. Phys. Chem.*, **2**, 273(1989) (Ch).
2. Liguoy Yi, **Shubin Liu**, Kanping Xu and Lixin Liu, "Cattell 16PF: measurement and research", *J. Hunan Normal Univ.*, **19**, 115(1990) (Ch).
3. **Shubin Liu** and Yuxin Yu, "A novel interpretation of Hund's rule for two-electron molecular systems", *J. Mol. Struct. THEOCHEM*, **235**, 115(1991).
4. **Shubin Liu**, Xiaoyu Liu, Qingsong Yang and Yuxin Yu, "The dominance of Hund's rule by the kinetic energy difference for molecular systems at all internuclear separations", *J. Mol. Struct. THEOCHEM*, **251**, 271(1991).
5. **Shubin Liu** and Zhouren Peng, "The internal polarization basis set: a note of the force-adapted *ab initio* calculation," *J. Chem. Phys.*, **94**, 4101(1991).
6. Hongxin Huang and **Shubin Liu**, "Variational quantum Monte Carlo methods and random number generators", *Chinese Bulletin of Science*, **38**, 1958(1993)(Ch).
7. Hongxin Huang and **Shubin Liu**, "Variational Monte Carlo treatment of molecules: a novel algorithm in terms of correlated sampling and Hartree-Fock approach", *J. Mol. Struct. THEOCHEM*, **312**, 281(1994).
8. Robert G. Parr, **Shubin Liu**, Alfred A. Kugler, and Ágnes Nagy, "Some identities in density functional theory", *Phys. Rev. A*, **52**, 969(1995).
9. **Shubin Liu** and Robert G. Parr, "Cusp relations for local strongly decaying properties in electronic systems", *Phys. Rev. A*, **52**, 2645(1995).
10. **Shubin Liu** and Robert G. Parr, "Expansion of correlation energy density functional and its kinetic component in terms of homogeneous functionals", *Phys. Rev. A*, **53**, 2211(1996).
11. Ágnes Nagy, Robert G. Parr, and **Shubin Liu**, "Local temperature in an electronic system", *Phys. Rev. A*, **53**, 3117(1996).
12. Pratim K. Chatteraji, Swapan K. Ghosh, **Shubin Liu**, and Robert G. Parr, "Exchange-correlation potential and excited-state density functional theory", *Int. J. Quantum Chem.*, **60**, 535(1996).
13. **Shubin Liu**, "Local density approximation, hierarchy of equations, functional expansion, and adiabatic connection in Current-Density-Functional Theory", *Phys. Rev. A*, **54**, 1328(1996).

14. **Shubin Liu**, Peter Süle, Roberto L. Boada, and Ágnes Nagy, "Application to atoms, ions, and molecules of a novel form of the correlation energy density functional", *Chem. Phys. Lett.*, **257**, 68(1996).
15. Zhong-Zhi Yang, **Shubin Liu**, and Yan A. Wang, "Uniqueness and asymptotic behavior of the local kinetic energy", *Chem. Phys. Lett.* **258**, 30(1996).
16. **Shubin Liu**, "Expansions of the pair distribution function and the second-order density matrix in terms of homogeneous functionals", *Phys. Rev. A.*, **54**, 4863(1996).
17. **Shubin Liu** and Robert G. Parr, "Expansions of density functionals in terms of homogeneous functionals: Justification and nonlocal representation of $T[\rho]$, $E_x[\rho]$, and $J[\rho]$ for atoms". *Phys. Rev. A*, **55**, 1792(1997).
18. Yan A. Wang, **Shubin Liu**, and Robert G. Parr, "Laurent series expansions in density functional theory". *Chem. Phys. Lett.*, **267**, 14(1997).
19. **Shubin Liu** and Robert G. Parr, "Second-order density functional description of molecules and chemical changes", *J. Chem. Phys.*, **106**, 5578 (1997).
20. Paul F. Heelis and **Shubin Liu**, "The photoenzymic repair of the DNA 6-4 photoproduct - a Density Functional and semiempirical study", *J. Am. Chem. Soc.*, **119**, 2936(1997).
21. Roberto Lopez-Boada, V. Karasiev, and **Shubin Liu**, "Padé approximation for the polynomial representation of the correlation energy density functional", *Chem. Phys. Lett.* **270**, 443(1997).
22. Frank De Proft, **Shubin Liu**, and Robert G. Parr, "Chemical potential, hardness, hardness and softness kernel and local hardness in the isomorphic ensemble of density functional theory", *J. Chem. Phys.* **107**, 3000(1997).
23. Robert G. Parr and **Shubin Liu**, "Some functional relations in the density functional theory of finite interacting electronic systems", *Chem. Phys. Lett.* **276**, 164(1997).
24. **Shubin Liu**, Frank De Proft, and Robert G. Parr, "Simplified models for the hardness kernel and calculations of global hardness", *J. Phys. Chem. A* **101**, 6991(1997).
25. **Shubin Liu** and Robert G. Parr, "Additional functional relations in the density functional theory of finite interacting electronic systems", *Chem. Phys. Lett.* **278**, 341(1997).
26. Robert G. Parr and **Shubin Liu**, "Consequences for finite electronic systems of possible homogeneity properties of density-functional energy components", *Chem. Phys. Lett.* **280**, 159(1997).
27. Hongxin Huang, Zexing Cao, and **Shubin Liu**, "Variance minimization for variational quantum Monte Carlo method, *Progress in Natural Science*, **7**, 549(1997).
28. Hongxin Hunag, Q.J. Xie, Zexin Cao, and **Shubin Liu**, "Hartree-Fock quantum Monte Carlo method", *Chinese Science Bulletin*, **42**, 1090(1997).
29. Wanhua Wang, Xiaoping Yang, and **Shubin Liu**, "Theoretical study of chlorosulfonyl isocyanate", *J. Xiangtan Normal Uni.*, **6**, 9(1997)(Ch).
30. Zhongzhi Yang, Yan A. Wang, and **Shubin Liu**, "On the single-electron local kinetic energy (I), *Sciences in China*, **27**(5), 268(1997)(Ch).
31. Zhongzhi Yang, Yan A. Wang, and **Shubin Liu**, "On the single-electron local kinetic energy (II), *Sciences in China Ser. B*, **41**, 174(1998).
32. Frank De Proft, **Shubin Liu**, and P. Geerlings, "Calculation of the nuclear Fukui function and new relations for nuclear softness and hardness kernels", *J. Chem. Phys.* **108**, 7549(1998).
33. **Shubin Liu**, Valentin Karasiev, Roberto L. Boada, and Frank De Proft, "Polynomial and Padi representations for the kinetic component of the correlation energy density functional", *Int. J. Quantum Chem.* **69**, 513(1998).
34. Wanhua Peng, **Shubin Liu**, and Xiaoping Yang, "Theoretical study of thiono-thiolo rearrangement in organophosphorus compounds", *Acta Chimica* **18**, 32(1998)(Ch).
35. Frank De Proft, P. Geerlings, **Shubin Liu**, and Robert G. Parr, "Variational calculation of the global hardness and the Fukui function via an approximation of the hardness kernel", *Polish J. Chem.* **72**, 1737(1998).

36. **Shubin Liu** and Robert G. Parr, "Consequences for the exchange energy density functional of the exponentially decaying nature of atomic electron density", *J. Comp. Chem.* **20**, 2(1999).
37. James P. Lewis, **Shubin Liu**, Lee Taisung, and Weitao Yang, "A Linear-Scaling Quantum Mechanical Investigation of Cytidine Deaminase", *J. Comp. Phys.* **151**, 242(1999).
38. **Shubin Liu**, Ágnes Nagy, and Robert G. Parr, "Expansion of the density functional energy components E_C and T_C in terms of moments of the electron density", *Phys. Rev. A* **59**, 1131(1999).
39. Robert G. Parr, Laszlo von Szentpaly, and **Shubin Liu***, "Electrophilicity index", *J. Am. Chem. Soc.* **121**, 192(1999).
40. Ágnes Nagy, **Shubin Liu**, and Robert G. Parr, "Expansion of the density functional energy components E_C and T_C in terms of moments of the electron density", *Phys. Rev. A* **59**, 3349(1999).
41. **Shubin Liu**, Paul W. Ayers, and Robert G. Parr, "A new exchange-correlation charge stemmed from the Zhao-Parr-Morrison method", *J. Chem. Phys.* **111**, 6197(1999).
42. **Shubin Liu**, Jose M. Pérez-Jordá, and Weitao Yang, "Nonorthogonal localized molecular orbitals in electronic structure theory", *J. Chem. Phys.* **112**, 1634(2000).
43. **Shubin Liu***, Frank De Proft, Agnes Nagy, and Robert G. Parr, "Exchange-energy density functionals as linear combination of homogeneous functionals of density", *Advances in Quantum Chemistry* **36**, 77(2000).
44. **Shubin Liu*** and Robert G. Parr, "Homogeneities in density of various LDA energy functionals", *J. Mol. Struct. THEOCHEM.* **501**, 29(2000).
45. Giuseppina Menconi, David J. Tozer, and **Shubin Liu**, "Atomic and molecular exchange-correlation charges in Kohn-Sham theory", *Phem. Chem. Chem. Phys.* **2**, 3739(2000).
46. Wilfried Langenaeker and **Shubin Liu**, "The response of atomic electron densities to point perturbations in the external potential", *J. Mol. Struct. THEOCHEM* **535**, 279(2001).
47. **Shubin Liu***, "Functional expansion approach in density functional theory", *Reviews of Quantum Chemistry*, World Scientific Press, pp 493-533, 2002.
48. **Shubin Liu***, "Recurrent generation of approximate functionals in density functional theory", *Int. J. Quantum Chem.* **90**, 282-290(2002)
49. Hongxin Huang and **Shubin Liu**, "Accurate fixed-node quantum Monte Carlo method", *J. Mol. Struct. THEOCHEM* **636**, 125-132(2003).
50. **Shubin Liu*** and Wilfried Langenaeker, "Hund's multiplicity rule: a unified interpretation", *Theor. Chem. Acc.* **110**, 338-344(2003).
51. **Shubin Liu*** and Paul W. Ayers, "Functional derivative of noninteracting kinetic energy density functional", *Phys. Rev. A* **70**, 022501-022505(2004).
52. Tonglei Li, **Shubin Liu**, Shaoxin Feng, and Clare E. Aubrey, "Face-Integrated Fukui Function: Understanding Wettability Anisotropy of Molecular Crystals From Density Functional Theory", *J. Am. Chem. Soc.* **127**, 1364-1365(2005).
53. Agnes Nagy, **Shubin Liu**, and Lee Bartllotti, "Generalized density functional theory for degenerate states", *J. Chem. Phys.* **122**, 134107(2005).
54. Aiguo Zhong and **Shubin Liu***, "Validity and interpretation of Hund's multiplicity rule for molecules: a density functional study", *J. Theor. Comp. Chem.* **4(3)**, 833-847(2005).
55. Yue Zeng, Jianlong Yi, Huixian Wang, Guzhen Zhou and **Shubin Liu**, "Theoretical study of $H_2PO_2^-$ adsorption on Ni(111) and Cu(111) surfaces", *J. Mol. Struct. THEOCHEM*, **724**, 81-86(2005).
56. Huang Hongxin and **Shubin Liu**, "An improved algorithm of fixed-node quantum Monte Carlo method with self-optimization process", *J. Mol. Struct. THEOCHEM* **726**, 93-97(2005).
57. **Shubin Liu***, "Dynamic behavior of chemical reactivity indices in density functional theory: A Bohn-Oppenheimer quantum molecular dynamics study", *J. Chem. Sci.* **117**, 477-83(2005).
58. Yue Zeng, **Shubin Liu**, Lihui Ou, Jianlong Yi, Shanci Yu, Huixian Wang and Xiaoming Xiao, "Density functional study of hypophosphite adsorption on Ni (1 1 1) and Cu (1 1 1) surfaces", *Appl. Surf. Sc.* **252**, 2692-2701(2006).

59. **Shubin Liu***, “Conditions for accurate description of the electron density of atoms and molecules”. *Int. J. Quantum Chem.* **106**, 1762-1768(2006).
60. Chunying Rong, Shixun Lian, Dulin Yin, Bin Shen, Aiguo Zhong, Lee Bartolotti, and **Shubin Liu***, “Towards understanding performance differences between approximate density functionals for spin states of iron complexes”, *J. Chem. Phys.* **125**, 174102(2006).
61. **Shubin Liu***, Robert C. Morrison, Robert G. Parr, “Approximate scaling properties of the DFT Tc for atoms”, *J. Chem. Phys.* **125**, 174109(2006).
62. Chunying Rong, Shixun Lian, Dulin Yin, Aiguo Zhong, Ruiqin Zhang, and **Shubin Liu***, “Effective simulation of biological systems: Choice of density functional and basis set for heme-containing complexes”, *Chem. Phys. Lett.* **434**, 149-154(2007).
63. W.J. Fan, Ruiqin Zhang, and **Shubin Liu***, “Computation of large systems with an economic basis set: Structures and reactivity indices of nucleic acid base pairs from density functional theory”, *J. Comp Chem.* **28**, 967-974(2007).
64. Joshua D. Sieber, **Shubin Liu**, and James P. Morken, “Catalytic Conjugate Addition of Allyl Groups to Styryl-Activated Enones”, *J. Am. Chem. Soc.* **127**, 2214-2215(2007).
65. Paul W. Ayers and **Shubin Liu**, “Necessary and Sufficient Conditions for the N-representability of Density Functionals”, *Phys. Rev. A* **75**, 022514(2007).
66. Aiguo Zhong, Chunying Rong, and **Shubin Liu***, "Structural and Dynamic Properties of (SiO₂)₆ Silica Nanostructures: A Quantum Molecular Dynamics Study", *J. Phys. Chem.A* **111**, 3132-3136(2007).
67. **Shubin Liu***, “On the relationship between Shannon entropy and Fisher information”, *J. Chem. Phys.* **126**, 191107 (2007).
68. Jennifer R. Weinberg-Wolf, Laura E. McNeil, **Shubin Liu** and Christian Kloc, “Evidence of low intermolecular coupling in rubrene single crystals by Raman scattering”, *J. Phys. Condens. Matter.* **19**, 276204 (2007).
69. **Shubin Liu***, “Steric effect: A quantitative description from density functional theory”, *J. Chem. Phys.* **126**, 244103 (2007).
70. Heather E. Burks, **Shubin Liu***, and James P. Morken, “Development, Mechanism, and Scope of the Palladium-Catalyzed Enantioselective Allene Diboration”, *J. Am. Chem. Soc.* **129**, 8766-8773(2007).
71. **Shubin Liu*** and Robert G. Parr, “Atomic correlation energy from the electron density at the nucleus”, *J. Phys. Chem. A*, **111**, 10422-10425(2007).
72. **Shubin Liu**, Lalith Perera, and Lee G. Pedersen, “Binuclear manganese (II) complexes in biological systems”, *Mol. Phys.* **105**, 2893-2898(2007).
73. Ying Huang, Aiguo Zhong, Chunying Rong, Xiaoming Xiao and **Shubin Liu***, “Structure, Spectroscopy, and Reactivity Properties of Porphyrin Pincers: A Conceptual DFT and TD-DFT Study”, *J. Phys. Chem. A* **112**, 305-311(2008).
74. Agnes Nagy and **Shubin Liu**, “Local wave-vector, Shannon and Fisher Information”, *Phys. Letts. A.* **372**, 1654-1656(2008).
75. **Shubin Liu*** and Niranjan Govind, “Towards Understanding the Nature of Internal Rotation Barriers with a New Energy Partition Scheme: Ethane and n-Butane”, *J. Phys. Chem. A* **112**, 6690-6699(2008).
76. Yue Chen, **Shubin Liu***, Ming Lei, “The Nature of Asynchronous Hydrogen Transfer in Ketone Hydrogenation Catalyzed by Ru Complex”, *J. Phys. Chem. C* **112**(35), 13524-13527(2008).
77. **Shubin Liu***, Niranjan Govind, and Lee G. Pedersen, “Towards Understanding Origin of Internal Rotational Barrier for Molecules with One Rotatable Dihedral Angle”, *J. Chem. Phys.* **129**, 094104(2008).
78. Yue Xia, Dulin Yin, Chunying Rong, Qiong Xu, Donghong Yin, and **Shubin Liu***, “Impact of Lewis acids on Diels-Alder Reaction Reactivity: A Conceptual Density Functional Theory Study”, *J. Phys. Chem. A* **112**, 9970-9977 (2008).
79. Qiang Chen, Yuanyuan Jia, **Shubin Liu**, Alfred Kleinhammes, and Yue Wu, “Molecules Immobilization in Titania Nanotubes: A Solid-State NMR and Computational Chemistry Study”,

J. Phys. Chem. C, **112**, 17331–17335(2008).

80. Ai-Guo Zhong, Dingben Chen, Ming Lei, and **Shubin Liu***, “Understanding the role of water in promoting E-isomer production and photochromism of solid schiff base: A DFT and TD-DFT study”, *J. Theor. Comp. Chem.* **7**, 1071-1084 (2008).

81. Tonglei Li, Paul W. Ayers, **Shubin Liu**, Matthew J. Swadley, Clare Aubrey-Medendorp, and Tonglei Li, “Crystallization Force - A Density Functional Theory Concept for Revealing Intermolecular Interactions and Molecular Packing in Organic Crystals”, *Chem. Euro. J.* **15**, 361-371(2009).

82. **Shubin Liu***, “Conceptual density functional theory and some recent developments”, *Acta Physico-Chimica Sinica* **25**, 590-600(2009).

83. **Shubin Liu**, “Electrophilicity”, Chapter 13 of the book “*Theory of Chemical Reactivity*”, edited by P.K. Chattaraj, published by Taylor and Francis Group, LLC, 2009.

84. Tang Zhi-Yong, Hu Yun-Chu, Zhao Yin, **Shubin Liu***, “Impact of Cyanoethy Groups on Structure and Spectroscopy of a Few Aromatic Amines: A Density Functional Theory and Time-Dependent Density Functional Theory Study”, *Acta Physico-Chimica Sinica*, **25**, 701-706(2009).

85. Miquel Torrent-Sucarrat, **Shubin Liu***, and Frank De Proft, “Steric Effect: Partitioning in Atomic and Functional Group Contributions”, *J. Phys. Chem. A* **113**, 3698–3702(2009).

86. Shixun Lian, Chunying Rong, Dulin Yin, and **Shubin Liu***, “Enhancing Solar Energy Conversion Efficiency: A Tunable Dual-Excitation Dual-Emission Phosphors and Time-Dependent Density Functional Theory Study”, *J. Phys. Chem. C* **113**, 6298–6302(2009).

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94. **Shubin Liu***, Tonglei Li, and Paul W. Ayers, “Potentialphilicity and potentialphobicity: Reactivity indicators for external potential changes from density functional reactivity theory”, *J. Chem. Phys.* **131**, 114106 (2009).

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114. Ying Huang, Ai-Guo Zhong, Qinsong Yang, and **Shubin Liu***, “Origin of Anomeric Effect: A Density Functional Steric Analysis”, *J. Chem. Phys.* **134**, 084103 (2011).
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117. Ying Huang, Aiguo Zhong, **Shubin Liu***, “Predicting pKa values for substituted benzoic acids with density functional reactivity theory”, *J. Nat. Sci. Hunan Normal Univ.* **34(1)**, 52-55(2011).
118. Pan-Pan Zhou, Wen-Yuan Qiu, **Shubin Liu**, and Neng-Zhi Jin, “Halogen as Halogen-Bonding Donor and Hydrogen-Bonding Acceptor Simultaneously in Ring-Shaped H₃N•X(Y)•HF (X=Cl, Br and Y=F, Cl, Br) Complexes”, *Phys. Chem. Chem Phys.* **113**, 7408-7418 (2011).
119. Sangwook Wu, **Shubin Liu**, Charles H. Davis, Darrel W. Staffordz, Lee G. Pedersen, “A heterodimer model for concerted action of vitamin K carboxylase (VKC) and vitamin K reductase (VKOR) in vitamin K cycle”, *J. Theoretical Biology* **279**, 143-149 (2011).
120. Rodolfo O. Esquivel, **Shubin Liu***, Juan Carlos Angulo, Jes´us S. Dehesa, Juan Antol´ın, and Moyocoyani Molina-Esp´ıritu, “Fisher Information and Steric Effect: A Study of the Internal Rotation Barrier of Ethane”, *J. Phys. Chem. A* **115**, 4406-4415 (2011).
121. Douglas Tsao, **Shubin Liu**, and Nikolay Dokholyan, “Regioselectivity of Catechol O-Methyltransferase Confers Enhancement of Catalytic Activity”, *Chem. Phys. Lett.* **506**, 135-138 (2011).
122. Samantha Jenkins, Chunying Rong, Steven Robert Kirk, Dulin Yin, **Shubin Liu***, “Spanning Set of Silica Cluster Isomer Topologies from AIM”, *J. Phys. Chem. A*, *in press*.
123. Jui-Hua Hsieh, Shuangye Yin, Xiang S. Wang, **Shubin Liu**, Nikolay V. Dokholyan, and Alexander Tropsha, “Cheminformatics Meets Molecular Mechanics: A Combined Application of Knowledge Based Pose Scoring and Physical Force Field-based Hit Scoring Functions Improves the Accuracy of Virtual Screening”, *J. Chem. Info. Model.* *submitted*.
124. J. R. Weinberg-Wolf, L. E. McNeil, **Shubin Liu** and Christian Kloc, “Temperature Dependent Photoluminescence Spectroscopy of Rubrene Single Crystals”, *J. Phys. Cond. Mat.* *submitted*.

INVITED TALKS

1. "Understanding protein folding in terms of the lattice model", Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina, Sept. 5, 1996.
2. "Alternative definition of exchange-correlation charge stemmed from the Zhao-Morrison-Parr method", 50th Southeast regional conference of American Chemical Society, Symposium in honor of Robert G. Parr, Research Triangle Park, North Carolina, November 4-7, 1998.
3. “Linear scaling methods in density functional theory: an implementation with non-orthogonal localized molecular orbital”, The 1st World Chinese Computational Chemistry Symposium, Dailian, Liaoning, China, August 15 – 18, 2000.
4. “Functional expansion approach in density functional theory”, 40th IUPAC Congress, Beijing, China., August 2005.
5. “Recent developments of concepts and theory in DFT”, City University of Hong Kong, China, August 2005.
6. “Density functional expansion and dynamic profiles of DFT indices”, University of Hong Kong, China, August, 2005.
7. “Quantum molecular dynamics and time profiles of density functional reactivity indices”, Symposium on Computational Chemistry and Parallel Software (CAS-SCCPS), Chinese Academy of Science, Zhangjiajie, Hunan, China, July 10 - 12, 2006.
8. “Density functional theory: Some recent developments”, Beijing Normal University, March 15, 2007.
9. “Density functional theory: Some recent developments”, Beijing University of Chemical Technology, March 18, 2007.
10. “Spin-related issues in DFT: Interpretation of Hund's multiplicity rule and density functional Performance for iron-containing complexes”, 2007 International Workshop on Frontiers of Theoretical & Computational Physics and Chemistry, Qingdao, China, August 10-12, 2007.

11. "Some recent developments of conceptual density functional theory", Hong Kong University of Science and Technology, Hong Kong, China, June 23, 2008.
12. "Is there a density functional theory for atoms and molecules", 2008 Symposium of Computational Chemistry and HPC Applications, Qingdao, China, June 29 – July 3, 2008.
13. "Quantification of electrophilicity and steric effect with DFT", 26th Chinese Chemical Society Congress, Tianjin, China, July 13-16, 2008.
14. "Research Computing at Carolina and Density Functional Reactivity Theory", Center of Computational Sciences, University of Kentucky, March 4, 2009.
15. "Conceptual Density Functional Theory", The 4th International Conference on Theoretical Chemistry, Molecular Modeling and Life Sciences, Changchun, China, July 28-31, 2009.
16. "Conceptual Density Functional Theory: Some Recent Developments", Department of Chemistry, Duke University, June 4, 2010.

PRESENTATIONS

1. "Force method in quantum chemistry and its application in chemical bonding theory study", the 6th International Congress of Quantum Chemistry, Israel, 1988.
2. "OOF (orbital overlap force) as a general bonding criterion", Symposium of Young Scientists, Hunan Normal University, Hunan, PRC, Nov., 1989.
3. "Orbital forces: decomposition and application", the 4th National Conference of Quantum Chemistry of China, Jinan, Shandong Province, PRC, Oct., 1990.
4. "Theoretical interpretation of Hund's rule for molecular systems", the 7th International Congress of Quantum Chemistry, Menton, France, July, 1991.
5. "On the magic number phenomenon of small carbon cluster ions: a theoretical consideration", the Science Association of Hunan Province, Hunan, PRC, Nov., 1992.
6. "Density Functional Theory in inhomogeneous simple fluids", Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina, Dec., 1994.
7. "Full dimensional time-dependent *ab initio* calculations for diatomic-diatom reactions: H₂+OH reaction", Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina, April, 1995.
8. "Toward finding the new generation of energy density functionals", Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina, Oct., 1995.
9. "A new local form of the correlation energy density functional", 25th Southeastern theoretical chemistry association conference, Florida State University, Tallahassee, Florida, May, 1996.
10. "Studies on Density Functional Theory: Functional expansion and a new form of the correlation energy density functional", Department of Chemistry, University of North Carolina, Chapel Hill, Sept. 30, 1996.
11. "Simplified Models for Computing Hardness", The 111th Conference of the North Carolina Section of the American Chemical Society, Durham, NC, April 5, 1997.
13. "Functional Expansion Approach in Density Functional Theory", The 213th National Conference of the American Chemical Society, San Francisco, CA, April 13, 1997.
14. "Second-Order Truncation Theorem in Density Functional Theorem and More", Department of Chemistry, University of North Carolina, Chapel Hill, NC, May 26, 1997.
15. "Functional Expansion Approach in Density Functional Theory", Symposium of Density Functional Theory, Duke University, Durham, NC, June 3, 1997.
16. "Density Functional Theory of the Hydrogen-Like System and the Local Exponential Approximation of Density", Department of Chemistry, Duke University, Durham, NC, December 15, 1997.
17. "Nonorthogonal localized molecular orbitals of electronic structure theory", The 40th Sanibel Symposium of Quantum Chemistry, St. Augustine, February 26 – March 3, 2000.
18. "Homology modeling, structure and dynamics of human cytochrom P450 protein 2D6", Gordon Research Conference on Protein Folding, Ventura, California, February 2002.

19. "QM/MM study of reaction mechanism of P450cam protein", Gordon Research Conference of Computational Chemistry, Holderness School, New Hampshire, July 2004.
20. "Optical characterization of single crystals of the organic semiconductor rubrene", 2005 APS March Meeting, March 21–25, 2005, Los Angeles, CA.
21. "Towards understanding performance differences between approximate density functionals for spin states of iron complexes", the 46th Sanibel Symposium, St. Simons Island, GA, March 3-7, 2006.
22. "A New Quantitative Structure-Activity Relationship Method using NMR Descriptors and Simulated Annealing/Principal Component Analysis Techniques", 2006 AAPS Annual Meeting and Exposition, October 31, 2006.
23. "Structure of Hydroquinone/Titania-nanoscroll Hybrid: NMR Experiments, X-ray Diffraction, Raman, and Quantum Chemical Calculations", 48th Experimental Nuclear Magnetic Resonance Conference, Daytona Beach, Florida, April 22-27, 2007.
24. "Asymmetric conjugate addition of allylboronates to activated enones using Ni-catalysis", the 234th ACS National Meeting, Boston, MA, August 19-23, 2007.
25. "Towards Understanding the Nature of Internal Rotation Barriers with a New Energy Partition Scheme: Ethane and n-Butane", the 48th Sanibel Symposium at the King and Prince Golf & Beach Resort on St. Simons Island, Georgia Feb. 20-26, 2008.
26. "A Combination of Target-specific Pose Filters and Force Field-based Scoring Functions to Improve the Structure-based Virtual Screening", ACS Spring National Meeting, San Francisco, CA, March 21 - 25, 2010.
27. "Quantification of Steric Effect in Density Functional Theory", the 50th Sanibel Symposium, St. Simons Island, GA, February 24 - March 3, 2010.
28. "Separation and Association Propensity of Proton and Electron Transfers: A Conceptual Density Functional Theory Characterization", the UNC EFRC First Annual Science Conference, UNC-CH, Chapel Hill, NC May 9-11, 2010.
29. "Understanding intermolecular interactions with density functional theory", Gordon Research Conference on Crystal Engineering, Waterville Valley, NH, June 6-11, 2010.
30. "Developing DFT concepts for characterizing intermolecular interactions in organic crystals", ACS National Conference, Boston, August 25, 2010.
31. "Density Functional Steric Analysis", the 51th Sanibel Symposium, St. Simons Island, GA, February 25 - March 2, 2011.

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