

## Curriculum Vitae

### Dr. Zhongfang CHEN

Dept. of Chemistry  
Department of Chemistry  
University of Puerto Rico  
San Juan, PR 00923, USA  
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### EDUCATION

- 1997.09 – 2000.7 Ph. D. in Physical Chemistry, Dept. of Chemistry, Nankai University, P. R. China  
Supervisor: Prof. Auchin Tang and Prof. Xuezhuan Zhao  
“Quantum Chemical Computations on Heterofullerens and Fullerene Derivatives”
- 1994.09 – 1997.07 M. S. in Physical Chemistry, Dept. of Chemistry, Nankai University, P. R. China,  
Supervisor: Prof. Xuezhuan Zhao  
“Preparation of Fullerenes and Synthesis of Fullerene Derivatives”
- 1990.09 – 1994.07 B. S. in Organic Chemistry, Dept. of Chemistry, Nankai University, P. R. China

### PROFESSIONAL EXPERIENCE

- 2008.8- Associate Professor, Department of Chemistry, University of Puerto Rico, Río Piedras campus
- 2008.1-2008.7 Research Associate Professor, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute
- 2006.1-2007.12 Associate Research Scientist, Department of Chemistry, University of Georgia
- 2003.10 – 2005.12 Postdoc, Department of Chemistry, Center for Computational Chemistry, University of Georgia, with Prof. Paul von Ragué Schleyer
- 2002.10 – 2003.9 Postdoc, Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany, with Prof. Andreas Hirsch and Prof. Paul von Ragué Schleyer
- 2001.04 – 2002.9 Humboldt Fellow, Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany, with Prof. Andreas Hirsch
- 2000.04 – 2001.03 Postdoc, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany, with Prof. Walter Thiel
- 1999.12 – 2000.02 Humboldt Fellow, Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany, with Prof. Andreas Hirsch

### TEACHING EXPERIENCE

- 2008.1 – 2008.5 Organizing the Condensed Matters and Optics Physics Graduate Student Seminar, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute
- 2003.10 – 2005.1 – 2005.5 Helping mentor graduate students of Prof. Schleyer group at University of Georgia  
Independent Instructor, Computational Chemistry (CHEM 8990, at graduate level), Department of Chemistry, University of Georgia
- 2004.8 – 2004.12 Guest lecturer, “Stereochemistry and Conformations” (CHEM 8300, at graduate level), Department of Chemistry, University of Georgia
- 1997.9 – 1998.1 Teaching Assistant, Advanced Physical Chemistry Experiment, Department of Chemistry, Nankai University
- 1995.9 – 1996.1 Teaching Assistant, Advanced Physical Chemistry Experiment, Department of Chemistry, Nankai University

### RECENT HONORS and AWARDS

- 2007 Short-term Fellowship, International Center for Young Scientists, National Institute for Materials Science, Tsukuba, Japan
- 1999 Max-Planck-Institute Postdoctoral Fellowship, Germany

- 1999 Alexander von Humboldt Fellowship, Germany
- 1999 Special-grade Scholarship of Nankai University (the highest prize that the students in Nankai University can be awarded within the university), P.R. China
- 1998 Yang Shixian Scholarship, Nankai University (the highest prize for the students in College of Chemistry in Nankai University), P.R. China
- 1996 Guanghua Fellowship, Nankai University, P.R. China
- 1994 Excellent Student Honor, Nankai University, P.R. China

## RECENT MAIN RESEARCH TOPICS

- One-dimensional nanomaterials (nanotubes, nanocables, peapods, etc)
- Novel materials for hydrogen and lithium storage
- Endohedral metallofullerenes and related endohedral clusters
- Molecules with novel bonding patterns
  - ✧ Planar hypercoordinate carbon and other elements
  - ✧ Novel aromaticity

## RESEARCH TOPICS BEING DEVELOPED

- Toxicity prediction of nanomaterials
- Photocatalysis and fuel cell

## PUBLICATIONS (see the publication-list for details)

- 100 publications, including *Chem. Rev.* (3), *J. Am. Chem. Soc.* (10), *Angew. Chem. Int. Ed.* (6) and *Phys. Rev. Lett.* (1).
- 49 first-authored, 35 correspondence-authored, total citation number 1723, h-index 24.
- Five papers were highlighted by news media (*Chem. & Eng. News* and/or *Nachrichten aus der Chemie*); four were highlighted as cover pictures of scientific journals (*ChemPhysChem*, *J. Comput. Chem.*, *J. Phys. Chem. A*, *J. Phys. Chem. C*); Two articles in *Chem. Rev.* were ranked as “hot paper”, “most-cited” or “most-accessed article” by ACS publications.

## PROFESSIONAL SERVICES

### Membership in Professional Associations

- American Chemical Society
- Alexander von Humboldt Association of America

### Evaluation of Manuscripts for Journals (29 international journals, around 40 manuscripts in 2007)

<i>J. Am. Chem. Soc.</i>	<i>Inorg. Chem.</i>	<i>Nanotechnology</i>	<i>J. Nanosc. &amp; Nanotech.</i>
<i>Nature Materials</i>	<i>ChemPhysChem</i>	<i>Chem. Phys. Lett.</i>	<i>J. Theor. Comp. Chem.</i>
<i>Chem. Eur. J.</i>	<i>Small</i>	<i>Carbon</i>	<i>Molecular Simulations</i>
<i>Org. Lett.</i>	<i>Phys. Rev. B</i>	<i>J. Mol. Mod.</i>	<i>Centr. Eur. J. Chem.</i>
<i>J. Phys. Chem. A</i>	<i>J. Chem. Phys.</i>	<i>J. Mol. Struct. (Theochem)</i>	<i>Int. J. Quant. Chem.</i>
<i>J. Phys. Chem. B</i>	<i>J. Comp. Chem.</i>	<i>Int. J. Mass Spect.</i>	<i>Mol. Phys.</i>
<i>Curr Opin Colloid Interface Sci</i>		<i>Physica Status Solidi</i>	<i>J. Mol. Graph. Mod</i>
<i>J. Phys. D</i>	<i>Physica E</i>		

### Evaluation of Research Proposals (3 funding agencies)

- National Science Foundation
- Department of Energy
- The U.S. Civilian Research and Development Foundation (CRDF)

### Member of the Organizing Committee of Conferences

- Nano and Giga Challenges in Electronics and Photonics From Atoms to Materials to Devices to System Architecture Symposium and Spring School, Phoenix, Arizona, March 12-16, 2007
- Workshop on Computational Nanoscience and New Energy Material, Tianjin, China, March 14-17,

2008

- Nano and Giga Challenges in Electronics, Photonics and Renewable Energy, Ontario, Canada, August 10-14, 2009

**INVITED CONFERENCE/SEMINAR TALKS (64)**

- Sept. 29 2008 Department of Physics, University of Science and Technology of China, Hefei, China  
Sept. 28 2008 Department of Physics, University of Science and Technology of China, Hefei, China  
Sept. 24 2008 **International Conference on Theory and Applications of Computational Chemistry, Shanghai, China**  
  
Sept. 19 2008 Institute for Metal Research, Shenyang National Lab, Shenyang, China  
Sept. 18 2008 College of Advanced Science and Technology, Dalian University of Technology, Dalian  
Sept. 16 2008 Department of Physics, Tsinghua University, Beijing, China  
Sept. 14 2008 The graduate school of Chinese Academy of Science, Beijing, China  
Apr. 8 2008 Department of Chemistry, University of Puerto Rico, Río Piedras Campus, Puerto Rico  
Mar. 17 2008 Institute of New Energy Material Chemistry, Nankai University, China  
Mar. 16 2008 **Workshop on Computational Nanoscience and New Energy Material, Tianjin, China**  
Mar. 6 2008 Department of Chemistry, Missouri University of Science and Technology, USA  
Mar. 11 2008 **Final Workshop of International Center for Young Scientists, National Institute for Materials Science, Tsukuba, Japan**  
  
Oct. 24 2007 Virtual Conference on Nanoscale Science and Technology, Fayetteville, AR, USA  
Jul. 26 2007 Young Research Talks, ICYS-ICMR Summer School on Nanomaterials, Tsukuba, Japan  
Jul. 17 2007 Department of Chemistry, University of Tsukuba, Tsukuba, Japan  
Jul. 6 2007 Department of Material Science, Kyushu University Fukuoka, Japan  
Jul. 2 2007 Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan  
Jun. 1 2007 International Center for Young Scientists, National Institute of Materials Science, Tsukuba, Japan  
  
Apr. 28 2007 **International Discussion Forum on Theoretical Catalysis and Materials Chemistry, Tainyuan, P. R. China**  
  
Apr. 12 2007 Brooklyn College, City University of New York, New York, USA  
Mar. 28 2007 Department of Chemistry, University of Texas at Arlington, Texas, USA  
Mar. 15 2007 **International Symposium “Nano and Giga Challenges in Electronics and Photonics”, Phoenix, Arizona, USA**  
  
Feb. 28 2007 Department of Chemistry, University of Nevada at Las Vegas, Las Vegas, USA  
Feb. 25 2007 Stony Brook University, New York, USA  
Feb. 9 2007 Department of Chemistry, University of Southern Mississippi, USA  
Nov. 1 2006 Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, USA  
Mar. 30 2006 231<sup>st</sup> ACS National Meeting, Atlanta, GA, USA  
Feb. 6 2006 Department of Chemistry and Biochemistry, Northern Illinois University  
Oct. 11 2005 Department of Chemistry, Clemson University, Clemson, SC, USA  
Jun. 17 2005 **1<sup>st</sup> NAREGI International Nanoscience Conference, Nara, Japan**  
Jun. 13 2005 National Institute for Materials Science, Advanced Materials Laboratory, Tsukuba, Japan  
Jun. 13 2005 Center for Tsukuba Advanced Research Alliance, University of Tsukuba, Tsukuba, Japan  
Jun. 10 2005 Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan  
Jun. 7 2005 Department of Chemistry, Nagoya University, Nagoya, Japan  
Jun. 6 2005 Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan  
May 23 2005 Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan  
May 18 2005 National Institute of Advanced Industrial Science and Technology (AIST), Osaka, Japan  
Nov. 11 2004 56th Southeast Regional Meeting of the ACS, Research Triangle Park, Durham, NC, USA  
Aug. 22 2004 **228th ACS fall meeting, Symposium in honor of Prof. H. F. Schaefer III's 60th birthday, Philadelphia, USA**  
  
Aug. 3 2004 **International Conference on Optoelectronics and Spectroscopy of Nano-Structured Thin Films and Materials, Beijing, China**  
  
Jul. 22 2004 Department of Physics and Astronomy, Katholieke Universiteit Leuven, Belgium  
Jul. 21 2004 Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, Germany  
Jul. 19 2004 Institute of Theoretical Physics, University of Paderborn, Germany

Jul. 16	2004	Institute of Organic Chemistry, University of Bochum, Germany
Jul. 6	2004	Institute of Organic Chemistry, University of Erlangen-Nuernberg, Germany
May 7	2004	Institute of Chemistry, Chinese Academy of Science, Beijing, P. R. China
May 5	2004	College of Chemistry, Nankai University, Tianjin, P. R. China
May 11	2004	Department of Chemistry, Tianjin Normal University, Tianjin, P. R. China
May 8	2004	Department of Chemistry, Xiamen Univ. P. R. China
Apr.	2004	Department of Chemistry, Peking University, Beijing, P. R. China
Mar.	2004	Emerson Center, Emory University, Atlanta, GA, USA
Nov.	2003	55th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, USA
May 3	2003	National Institute of Advanced Industrial Science and Technology (AIST), Osaka, Japan
Apr. 5	2003	Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan
Sep. 24	2002	Max-Planck-Institut fuer Kohlenforschung, Muelheim an der Ruhr, Germany
Sep.18	2002	Institut fuer Organische Chemie, Univ. of Kiel, Kiel, Germany
May 13	2002	Theoretical Chemistry Institute, University of Heidelberg, Heidelberg, Germany
Feb.	2002	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
Feb.	2002	Institut fuer Physikalische Chemie, Technische Universität Dresden, Dresden, Germany
Dec.	2001	Department of Chemistry, Nankai Univ., Tianjin, P. R. China
Dec.	2001	Institute of Coal Research, Tainyuan, P. R.China
Dec.	2001	<b>International Symposium of Clean Coal Utilization, Sanya, P. R. China</b>
Apr.	2001	Department of Chemistry, Nankai Univ., Tianjin, P. R. China
Dec.	2000	Department of Physics, Fudan University, Shanghai, P. R. China

#### **VISITING EXPERIENCES (Duration More than One Month)**

May-Jul.	2007	International Center for Young Scientists, National Institute for Materials Science, Tsukuba, Japan
May	2005	Institute for Molecular Science, Okazaki, Japan
Jul. – Aug.	2004	Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr
Jun. – Jul.	2004	Institut für Organische Chemie, Universität Erlangen-Nürnberg, Germany
Apr. – May	2003	Institute for Molecular Science, Okazaki, Japan
Feb.	2002	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.

#### **PROFESSIONAL REFERENCES**

- Prof. Paul von Ragué Schleyer  
Dept. of Chemistry, Center for Computational Chemistry, University of Georgia, Athens, GA 30602  
Email: [schleyer@chem.uga.edu](mailto:schleyer@chem.uga.edu) Tel: 706-542-7510;
- Prof. Henry Schaefer III  
Center for Computational Chemistry, University of Georgia, Athens, GA 30602 USA  
Email: [hfs@uga.edu](mailto:hfs@uga.edu) Tel: 706-542-0364; Fax: 706-542-0406
- Prof. Andreas Hirsch  
Institut für Organische Chemie, Universität Erlangen-Nürnberg, Erlangen, 91054 Germany  
Email: [andreas.hirsch@chemie.uni-erlangen.de](mailto:andreas.hirsch@chemie.uni-erlangen.de) Tel: +49 9131 85 22537; Fax: +49 9131 85 26864
- Prof. Shigeru Nagase  
Dept. of Theoretical Molecular Science, Institute for Molecular Science, Okazaki, 444-8585, Japan  
Email: [nagase@ims.ac.jp](mailto:nagase@ims.ac.jp) Tel: +81-564-55-7300 ; Fax: +81-564-53-4660
- Prof. Walter Thiel  
Max-Planck-Institut für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany  
E-mail: [thiel@mpi-muelheim.mpg.de](mailto:thiel@mpi-muelheim.mpg.de) Tel. +49208-306-2150; Fax +49-208-306-2996

## PUBLICATIONS OF DR. ZHONGFANG CHEN

### Statistics (Dec. 22, 2008)

Journal	Number	Journal	Number	Journal	Number
<i>Chem. Rev.</i>	3	<i>Inorg. Chem.</i>	2	<i>J. Phys. Org. Chem.</i>	1
<i>J. Am. Chem. Soc.</i>	10	<i>J. Comput. Chem.</i>	3	<i>Eur. J. Phys. D.</i>	1
<i>Angew. Chem. Int. Ed.</i>	6	<i>J. Chem. Phys.</i>	2	<i>Can. J. Chem.</i>	1
<i>Phys. Rev. Lett.</i>	1	<i>Chem. Mater.</i>	1	<i>J. Comput. Theor. Nanosci.</i>	2
<i>Chem. Eur. J.</i>	2	<i>Phys. Rev. B</i>	1	<i>Theochem</i>	4
<i>ChemPhysChem</i>	2	<i>Nanotechnology</i>	1	<i>Chem. J. Chin. Univ.</i>	6
<i>Org. Lett.</i>	1	<i>Chem. Phys. Lett.</i>	3	<i>Acta Chimica Sinica</i>	2
<i>J. Org. Chem.</i>	3	<i>J.C.S Faraday Trans</i>	1	<i>Polish J. Chem.</i>	1
<i>Organometallics</i>	2	<i>Phys. Chem. Chem. Phys.</i>	2	<i>Book chapter</i>	4
<i>J. Phys. Chem. A</i>	7	<i>Theor. Chem. Acc.</i>	2	<i>Others</i>	11
<i>J. Phys. Chem. B</i>	3	<i>J. Mol. Mod.</i>	3		
<i>J. Phys. Chem. C</i>	3	<i>Eur. J. Inorg. Chem.</i>	1		
Total	100				
First authored	49				
Correspondence authored	35				
Total number of citations	1723				
h-index	24				

### Selected Publications (10)

(\* indicates the corresponding authorship; citation numbers are also given for each paper)

10. Yafei Li, Zhen Zhou, Shengbai Zhang, **Zhongfang Chen\***  
MoS<sub>2</sub> Nanoribbons: High Stability, Unusual Electronic and Magnetic Properties  
*J. Am. Chem. Soc.* **2008**, *130*, 16739.
9. **Zhongfang Chen,\*** Sven Neukermans, Xin Wang, Ewald Janssens, Zhen Zhou, Roger E. Silverans, R. Bruce King, Paul v. R. Schleyer, Peter Lievens  
To Achieve Stable Spherical Clusters: General Principles and Experimental Confirmations  
*J. Am. Chem. Soc.* **2006**, *128*, 12829. [23 citations]
8. **Zhongfang Chen,\*** Chaitanya S. Wannere, Clémence Corminboeuf, Ralph Puchta, Paul. v. R. Schleyer  
Nucleus-Independent Chemical Shifts (NICS) as an Aromaticity Criterion  
*Chem. Rev.* **2005**, *105*, 3842. [252 citations]  
*Ranked as No. 1 "hot paper" of Chemical Reviews in January, 2008 by ACS publications as recognized by Thomson ISI®'s Essential Science Indicators (former rankings in 2007 were No. 21 in Jan, No. 18 in March, No. 13 in May, No. 12 in July, No. 5 in Sept. and No. 3 in Nov.)*
7. Xin Lu, **Zhongfang Chen\***  
Curved  $\pi$ -conjugation, Aromaticity and the Related Chemistry of Small Fullerenes (<C<sub>60</sub>) and Single-Walled Carbon Nanotubes  
*Chem. Rev.* **2005**, *105*, 3643. [95 citations]  
*Most-Accessed Article: October-December, 2005*
6. Xin Lu, **Zhongfang Chen,\*** Walter Thiel, Paul v. R. Schleyer, Rongbin Huang, Lansun Zheng  
Properties of Fullerene[50] and D<sub>5h</sub> Decachlorofullerene[50]: A Computational Study  
*J. Am. Chem. Soc.* **2004**, *126*, 14871. [55 citations]
5. **Zhongfang Chen,\*** Shigeru Nagase, Andreas Hirsch, Robert C Haddon, Walter Thiel, Paul v. R. Schleyer

- Side-Wall Opening of Single-Wall Carbon Nanotubes (SWCNTs) by Chemical Modification: A Critical Theoretical Study  
*Angew Chem. Int. Ed.* **2004**, *43*, 1552. [44 citations]
4. **Zhongfang Chen**,\* Andreas Hirsch, Shigeru Nagase, Walter Thiel, Paul v. R. Schleyer  
 Spherical Sila- and Germa-Homoaromaticity  
*J. Am. Chem. Soc.* **2003**, *125*, 15507. [21 citations]  
 Highlighted by  
*Chemical & Engineering News (C&EN)* (2004, March 1, page 29)  
*Chemical & Engineering News (C&EN)* (2003, Dec. 15, Page 26)
  3. **Zhongfang Chen**, Clémence Corminboeuf, Thomas Heine, Jon Bohmann, Paul v. R. Schleyer  
 Do All-Metal Antiaromatic Clusters Exist?  
*J. Am. Chem. Soc.* **2003**, *125*, 13930. [59 citations]  
 Highlighted by  
*Chemical & Engineering News (C&EN)* (2003, Dec. 15, Page 23-26)  
*Nachrichten aus der Chemie* (2003, Feb, page 121)  
 reported in Chemistry Highlights of 2003 (C&EN) (2003, Dec. 22, page 45)
  2. **Zhongfang Chen**, Haijun Jiao, Andreas Hirsch, Paul v. R. Schleyer  
 Spherical Homoaromaticity  
*Angew. Chem. Int. Ed.* **2002**, *41*, 4309. [24 citations]
  1. Andreas Hirsch, **Zhongfang Chen**, Haijun Jiao  
 Spherical Aromaticity in  $I_h$ -Symmetrical Fullerenes: the  $2(N+1)^2$  Rule  
*Angew. Chemie. Int. Ed.* **2000**, *39*, 3915. [105 citations]

### Full Publication List (100)

(\* indicates the corresponding authorship; citation numbers are also given for each paper)

#### A. Invited Reviews and Book Chapters

9. Zhen Zhou, Xin Lu, **Zhongfang Chen**\*  
 Curvature, Aromaticity and Reactivity of Carbon Nanotubes  
*Book chapter in Chemistry of Carbon Nanotubes*, edited by Prof. Vladimir A. Basiuk, American Scientific Publishers, 2007, page 47-73.
8. **Zhongfang Chen**,\* R. Bruce King  
 The Evaluation of Aromaticity in Inorganic Clusters and Related Compounds by Nucleus-Independent Chemical Shifts  
*ChemTracts-Inorganic Chemistry*, **2006**, *19*, 45.
7. Xin Lu, **Zhongfang Chen**\*  
 Curved  $\pi$ -Conjugation, Aromaticity and the Related Chemistry of Small Fullerenes (< $C_{60}$ ) and Single-Walled Carbon Nanotubes  
*Chem. Rev.* **2005**, *105*, 3463. [95 citations]  
*Most-Accessed Article: October-December, 2005*
6. **Zhongfang Chen**,\* R. Bruce King  
 Spherical Aromaticity: Recent Work on Fullerenes, Polyhedral Boranes, and Related Structures  
*Chem. Rev.* **2005**, *105*, 3613. [60 citations]
5. **Zhongfang Chen**,\* Chaitanya S. Wannere, Clémence Corminboeuf, Ralph Puchta, Paul. v. R. Schleyer  
 Nucleus-Independent Chemical Shifts (NICS) as an Aromaticity Criterion  
*Chem. Rev.* **2005**, *105*, 3842. [252 citations]  
*Ranked as No. 1 "hot paper" of Chemical Reviews in Jan., 2008 by ACS publications as recognized by Thomson ISI®'s Essential Science Indicators (former rankings in 2007 were No. 21 in Jan, No. 18 in March, No. 13 in May, No. 12 in July, No. 5 in Sept. and No. 3 in Nov.), the most- cited article*
4. Chaitany S. Wannere, **Zhongfang Chen**, Paul v. R. Schleyer  
 "Neutral" and "Anionic" Carbocations  
*Book chapter in hydrocarbon*, edited by Prof. G. A. Olah. 2004, Page 43-71.
3. **Zhongfang Chen**, Thomas Heine, Paul v. R. Schleyera, Dage Sundholm  
 Aromaticity Indices from Magnetic Shieldings  
*Book chapter in Calculation of NMR and EPR Parameters. Theory and Applications.* edited by M.

- Kaupp, M. Buehl and V. G. Malkin, Wiley-VCH, 2004. Page 395-407.
2. **Zhongfang Chen**, Haijun Jiao, Andreas Hirsch  
Spherical Aromaticity- An Overview  
*Book Chapter* in Developments in Fullerene Science (Fullerenes: From Synthesis to Optoelectronic Properties), edited by Dirk M. Guldi and Nazario Martin, KLUWER Academic publisher, 2002, Page 121-135.
  1. **Zhongfang Chen**, Xuezhuan Zhao, Auchin Tang  
Recent Progress on the Theoretical Studies of Heterofullerenes  
*Chinese Journal of Structural Chemistry* **1999**, *18*, 463. (in Chinese) [3 citations]
- B. Publications in Peer-Reviewed Journals**
91. Lu Wang, Jijun Zhao, Zhen Zhou, S. B. Zhang, **Zhongfang Chen\***  
First-Principles Study of Molecular Hydrogen Dissociation on Doped Al<sub>12</sub>X (X= B, Al, C, Si, P, Mg, Ca) Clusters  
*J. Comp. Chem.* **2008**, Accepted
  90. Yafei Li, Zhen Zhou, Shengbai Zhang, **Zhongfang Chen\***  
MoS<sub>2</sub> Nanoribbons: High Stability, Unusual Electronic and Magnetic Properties  
*J. Am. Chem. Soc.* **2008**, *130*, 16739.
  89. Lian Sun, Yafei Li, Zhenyu Li, Qunxiang Li, Zhen Zhou, **Zhongfang Chen**, Jinlong Yang, J. G. Hou  
Electronic Structures of SiC Nanoribbons  
*J. Chem. Phys.* **2008**, *129*, 174114.
  88. Yanyan Liu, Peiju Yang, Jie Yu, Xiao-Juan Yang, Jun D. Zhang, Zhongfang Chen, Henry F. Schaefer III, Biao Wu  
Sodium and Magnesium Complexes with Dianionic  $\alpha$ -Diimine Ligands  
*Organometallics* **2008**, ASAP, 10.1021/om800554q
  87. **Zhongfang Chen,\*** Haijun Jiao, Judy I. Wu, Rainer Herges, S. B. Zhang, Paul von Ragué Schleyer  
Homobenzene: Homoaromaticity and Homoantiaromaticity in Cycloheptatrienes  
*J. Phys. Chem. A* **2008**, *112*, 10586
  86. Zhen Zhou, Yafei Li, Lu Liu, Yongsheng Chen, S. B. Zhang, **Zhongfang Chen\***  
Size- and Surface-Dependent Stability, Electronic Properties, and Potential as Chemical Sensors: Computational Studies on One-Dimensional ZnO Nanostructures  
*J. Phys. Chem. C* **2008**, *112*, 13926.
  85. Xingfa Gao, Zhen Zhou, Yuliang Zhao, Shigeru Nagase, S. B. Zhang, **Zhongfang Chen \***  
Comparative Study of Carbon and BN Nanographenes: Ground Electronic States and Gap Energy Engineering  
*J. Phys. Chem. C* **2008**, *112*, 12677  
Highlighted  
as cover picture of *J. Phys. Chem C*. (Aug. 21, 2008)
  84. J. David Zhang, **Zhongfang Chen**, Henry F. Schaefer III  
Electron Attachment to the Hydrogenated Watson-Crick Guanine Cytosine Base Pair (GC+H): Conventional and Proton Transferred Structures  
*J. Phys. Chem. A* **2008**, *112*, 6217. .
  83. Jinlan Wang, Xiuyun Zhang, Paul von Ragué Schleyer, **Zhongfang Chen\***  
Density Functional Theory Studies of Inorganic Metallocene Multi-decker V<sub>n</sub>(P<sub>6</sub>)<sub>n+1</sub> (n = 1-4) Sandwich Clusters  
*J. Chem. Phys.* **2008**, *128*, 104706.
  82. J. David Zhang, **Zhongfang Chen**, R. Bruce King, Henry F. Schaefer III  
Comparison of Isoelectronic Heterometallic and Homometallic Binuclear Cyclopentadienylmetal Carbonyls: The Iron-Nickel versus the Dicobalt Systems  
*Eur. J. Inorg. Chem.*, **2008**, 1219.
  81. Zhen Zhou, Jijun Zhao, Paul v. R. Schleyer, **Zhongfang Chen\***  
Insertion of C<sub>50</sub> into Single-Walled Carbon Nanotubes: Selectivity in Interwall Spacing and C<sub>50</sub> Isomers  
*J. Comput. Chem.* **2008**, *29*, 781
  80. Xiaolan Zhou, Jijun Zhao, Xiaoshuang Chen, Wei Lu, Ruihua Xie, **Zhongfang Chen**, R. Bruce King  
From molecules to nanoscale materials: the structural and electronic properties of small gallium arsenide

- clusters up to Ga<sub>9</sub>As<sub>9</sub>  
*J. Comput. Theor. Nanosci.* **2008**, *5*, 70.
- 79 Yafei Li, Zhen Zhou, Dmitri Golberg, Yoshio Bando, Paul v. R. Schleyer, **Zhongfang Chen\***  
 Stone-Wales Defects in Single-Walled BN Nanotubes-Formation Energies, Electronic Structures and Reactivity  
*J. Phys. Chem. C.* **2008**, *112*, 1365. [1 citation]
- 78 Zhi-Xiang Wang, Cheng-Gen Zhang, **Zhongfang Chen**, Paul v. R. Schleyer  
 Planar Tetracoordinate Carbon Species Involving Beryllium  
*Inorg. Chem.* **2008**, *47*, 1332.
- 77 **Zhongfang Chen,\*** De-en Jiang, Xin Lu, Holger F. Bettinger, Sheng Dai, Paul v. R. Schleyer, Kendall N. Houk  
 Open-Shell Singlet Character of Cyclacenes and Short Zigzag Nanotubes  
*Org. Lett.* **2007**, *9*, 5449. [9 citation]
- 76 Sven Neukermans, Nele Veldeman, Ewald Janssens, Peter Lievens, **Zhongfang Chen**, Paul v. R. Schleyer  
 Combined Experimental and Theoretical Study of Small Aluminum Oxygen Clusters  
*Eur. J. Phys. D.* **2007**, *45*, 301.
75. Zhen Zhou, Jijun Zhao, Yongsheng Chen, Paul v. R. Schleyer, **Zhongfang Chen\***  
 Energetics and Electronic Structures of AlN Nanotubes/Wires and their Potential Application as Ammonia Sensors  
*Nanotechnology* **2007**, *18*, 424023. [5 citation]
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