

Sean C. Smith

Director
Center For Nanophase Materials Sciences Division
Oak Ridge National Laboratory
(865) 574-5081
smithsc@ornl.gov



Education

The University of Canterbury, New Zealand	Physical Chemistry	B.Sc. Hons, 1985
The University of Canterbury, New Zealand	Theoretical Chemistry	Ph.D., 1989

Professional Experience (ORNL = Oak Ridge National Laboratory; UQ = The University of Queensland)

2011/7 –	Director, Center for Nanophase Materials Sciences Division, ORNL
2002/11 – 2011/7	Professor of Computational Molecular Science, UQ; Director, Centre for Computational Molecular Science, UQ;
2006–2011/7	Group Leader for Computational Bio and Nanotechnology, Australian Institute for Bioengineering and Nanotechnology, UQ.
2003–2010	Program Leader and Deputy Director, Australian Research Council Centre of Excellence for Functional Nanomaterials.
1993/10–2002/11	Lecturer, Senior Lecturer and subsequently Associate Professor, Chemistry Department, UQ
1991–1993	Visiting Scholar, University of California-Berkeley
1989–1991	Alexander von Humboldt Research Fellowship, University of Göttingen, Germany

Professional and Synergistic Activities

2010–2012	Editor, Journal of Physical Chemistry
2003–present	Editor, Computer Physics Communications
2003–present	Australian Representative, International Union of Pure and Applied Chemistry (IUPAC) Physical and Biophysical Chemistry Divisional Committee (Nominated by Australian Academy of Science, elected at IUPAC General Assembly)

Honors and Awards

2007	Bessel Research Award of the Alexander von Humboldt Foundation, Germany
1999	FRACI, Fellowship of the Royal Australian Chemical Institute
1998	Le Fevre Memorial Prize, Australian Academy of Science
1998	Senior Visiting Fellowship, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan
1997	French Ministry of Higher Education and Research Senior Scientist Fellowship, France
1997	Alexander von Humboldt Foundation Visiting Scientist, Freiburg
1994	Rennie Memorial Medal, Royal Australian Chemical Institute
1989 – 1991	Alexander Von Humboldt Research Fellowship, Alexander von Humboldt Foundation, Federal Republic of Germany

Publications (Over 189 publications including 1 book, 3 invited book chapters, 5 invited reviews)
Full publication list follows CV.

Research Synopsis

1. *Fluorescent Proteins: Photophysics, Mechanism and Dynamics.*
We use electronic structure calculations (both cluster models and QM/MM for whole proteins), molecular and quantum dynamics to explore photophysical and dynamical processes in fluorescent proteins.
2. *Nanoparticle/Dendrimer Complexation with DNA and RNA for Gene Delivery and Gene Therapy applications.*
Molecular dynamics simulations are used to explore structure and stability of Layered Double Hydroxide nanoparticles and peptide-based dendrimers complexing with short DNA and RNA strands in aqueous solution, directed towards a knowledge-based approach to optimizing the efficiency of gene delivery to cells.
3. *Nanotubes and Nanoribbons: Reactivity, Functionalization and Electronics.*
We use electronic structure calculations and ab initio molecular dynamics to explore structure, reactivity and electronic properties of nanotube and nanoribbon systems, with and without functionalisation.
4. *Nanocomposite Materials for Hydrogen Storage.*
We use solid state electronic structure calculations and structure/kinetics models to elucidate catalytic mechanisms of hydrogen ad/absorption and desorption in designed nanocomposite materials.
5. *Metal Oxide Nanoparticles for Photocatalytic and Photovoltaic Applications.*
We are modelling electronic structure and surface interactions of metal oxide nanoparticles of great interest for photocatalysis (solar to hydrogen conversion) and photovoltaic applications. In particular we have focused recently on factors which allow the control of morphology and surface reactivity in anatase titania single crystals, as well as doping strategies to extend optical absorption from the UV out into the visible region.
6. *Novel membrane materials for CO₂ gas separation.*
Quantum chemical calculations and ab initio molecular dynamics are used to explore the interactions of small gaseous species such as CO₂, N₂, H₂O, CH₄ and H₂ with different nanotube architectures in order to assess the degree of selectivity for CO₂ that can be achieved.
7. *Quantum Kinetics of Hydrogen Transport in Confined Systems.*
We are simulating quantum transport of confined molecular hydrogen in meso- and nanoporous solids with immediate applications in the area of molecular sieving for separation of hydrogen from deuterium.
8. *Quantum Dynamics for Gas Phase Unimolecular Reactions.*
Quantum wavepacket methods are used to compute state-to-state reaction probabilities and thermal kinetics in key reactions for combustion and atmospheric science, e.g., HO₂ and HOCl.

Graduate and Postdoctoral Advisors

Past Ph.D. Students

S. Jeffreys; A. Rasmussen; T. Frankcombe; L. Kettle; S. Windsor; R. Gollan; D. Ouyang;
B. Wannoo; K. Wong; H. Yang

Current Ph.D. Students

Y. Jiao, P. Yao, University of Queensland, Y. Y. Ma, Beijing Normal University

Postdoctoral Associates

A. Du, T. Liao, M. Hankel, C. Sun, Q. Sun, University of Queensland

PUBLICATIONS

Sean C. Smith, Ph.D.

Center for Nanophase Materials Sciences Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831
smithsc@ornl.gov

Books

1. R.G. Gilbert and S.C. Smith, "Theory of Unimolecular and Recombination Reactions," 356pp, Blackwell Scientific Publications, Oxford, 1990.

Invited Chapters

3. H. Zhang, Q. Sun, S. Wang, S. Olsen and S.C. Smith, "Theoretical Studies of Green and Red Fluorescent Proteins," in "Hydrogen Bonding and Transfer in the Excited State," pp815-835, Eds. Ke-Li Han and Guang-Jiu Zhao, (Wiley, New York, 2011).
2. S.C. Smith, "Recent Developments in Statistical Rate Theory for Unimolecular and Complex-Forming Reactions," pp291-328 in *Modern Trends in Chemical Reaction Dynamics*, vol I, Xueming Yang and Kopin Liu eds. (World Scientific, Singapore, 2004).
1. S.C. Smith, "Unimolecular Reaction Dynamics," in *Encyclopedia of Computational Chemistry*, vol 4, H.F. Schaefer III ed. (Wiley, New York, 1998).

Invited Reviews

5. A. Du and S.C. Smith, "Electronic Functionality in Graphene-based Nanoarchitectures: Discovery and Design via First-principles Modeling," *J. Phys. Chem. Lett.*, **2**(2), (featured on front cover), 73-80 (2011).
4. C. Sun, L.M. Liu, A. Selloni, G.Q. Lu, S.C. Smith, "Titania-water Interactions: A Review of Theoretical Studies," *J. Mat. Chem.*, **20**, 10319-10334 (2010).
3. S.C. Smith, "Computational Studies Shed Light on Catalysis for Hydrogen Storage," *Materials Australia*, November/December edition pp36-38 (2006).
2. H. Zhang and S.C. Smith, "Recent Developments in the Quantum Dynamical Characterization of Unimolecular Resonances," *Phys. Chem. Chem. Phys.* (front cover feature), **6**, 884-894 (2004).
1. H. Zhang and S.C. Smith, "Quantum Dynamical Characterization of Unimolecular Resonances," *Phys. Chem. Comm.* (invited review article), **6**, 12-20 (2003).

Refereed Journal Papers (Thematically Grouped)

For full chronological listing see below, p13.

Papers are arranged in broad thematic areas.

Invited papers marked with an asterisk.

Journals with impact factor above 4 are highlighted in blue.

COMPUTATIONAL NANOTECHNOLOGY

180. C.H. Sun, A. Selloni, A. Du and S.C. Smith, "Interaction of Water with Fluorine-covered Anatase TiO₂ (001) Surface," *J. Phys. Chem. C* (accepted, August 2011).
178. A. Mukherjia, C.H. Sun, S.C. Smith, G.Q. Lu and L.Z. Wang, "Photocatalytic Hydrogen Production from Water Using N-doped Ba₅Ta₄O₁₅ Under Solar Irradiation," *J. Phys. Chem. C* (accepted, June 2011).
176. Y. Jiao, A. Du, Z.H. Zhu, V. Rudolph, G.Q. Lu and S.C. Smith, "A Density Functional Theory Study on CO₂ Capture and Activation by Graphene-like Boron Nitride with Boron Vacancy," *Catalysis Today* (accepted, March 2011).
175. C.H. Sun, Y. Wang, J. Zou and S.C. Smith "A Formation Mechanism of Oxygen Vacancies in a MnO₂ Monolayer: A DFT + U Study," *Phys. Chem. Chem. Phys.*, (accepted, Apr 2011).
174. A. Du, Y.H. Ng, N. Bell, Z.H. Zhu, R. Amal and S.C. Smith, "Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole-doping and Sensitization for Visible Light Response," *J. Phys. Chem. Lett.*, (accepted, Mar 2011).
173. N. Bell, Y.H. Ng, A. Du, H. Coster, S.C. Smith and R. Amal, "Understanding the Enhancement in Photoelectrochemical Properties of Photocatalytically-prepared TiO₂-Reduced Graphene Oxide Composite," *J. Phys. Chem. C*, accepted (February, 2011).
172. M. Hankel, H. Zhang, T.X. Nguyen, S.K. Bhatia, S.K. Gray, and S.C. Smith, "Kinetic Modelling of Molecular Hydrogen Transport in Microporous Carbon Materials," *Phys. Chem. Chem. Phys.*, **13**, 7834-7844 (2011).
171. X. Zong, C.H. Sun, Z.G. Chen, A. Mukherji, R. Gilbert, H. Wu, J. Zou, S.C. Smith, G.Q. Lu and L.Z. Wang, "Nitrogen Doping in Ion-Exchangeable Layered Tantalate towards Visible-Light Induced Water Oxidation," *Chem. Comm.*, accepted (February, 2011).
170. C.H. Sun, A. Mukherji, G.Q. Liu, L. Wang and S.C. Smith, "Improved Visible Light Absorption Of Htawo₆ Induced by Nitrogen Doping: An Experimental and Theoretical Study," *Chem. Phys. Lett.*, **501**, 427-430 (2010).
169. R. Marschall, A. Mukherji, A. Tanksale, C.H. Sun, S.C. Smith, G.Q. Lu, L.Z. Wang, "Preparation of New Sulfur-doped and Sulfur/Nitrogen Co-doped CsTaWO₆ Photocatalysts for Hydrogen Production from Water Under Visible Light," *J. Mat. Chem.*, (accepted December 2010).
167. Z. Li, X. Ma, Q. Sun, Z. Wang, J. Liu, Z.H. Zhu, S.Z. Qiao, S.C. Smith, G.Q. Lu and A. Mews, "Synthesis and Characterization of Colloidal Core-Shell Semiconductor Nanowires," *Eur. J. Inorg. Chem.*, **2010** (27), 4325-4331 (2010).
166. Y. Jiao, A. Du, Z. Zhu, V. Rudolph and S.C. Smith "A Density Functional Theory Study of CO₂ and N₂ Adsorption on Aluminium Nitride Single Walled Nanotubes," *J. Mat. Chem.*, **20**, 10426-10430 (2010).
165. A. Mukherji, R. Marschall, A. Tanksale, C.H. Sun, S.C. Smith, G.Q. Lu, L.Z. Wang, "N-doped CsTaWO₆ as a New Photocatalyst for Hydrogen Production from Water splitting under Solar Irradiation," *Adv. Funct. Mat.*, **21** (1), 126-132 (2010).

164. G. Liu, P. Niu, C.H. Sun, S.C. Smith, Z.G. Chen, G.Q. Lu and H.M. Cheng, "Unique Electronic Structure Induced High Photoreactivity of Sulfur-Doped Graphitic C₃N₄," *J. Amer. Chem. Soc.*, **132**(33), 11642-11648 (2010).
163. C.H. Sun, X.H. Yang, J.S. Chen, Z. Li, X.W. Lou, C.Z. Li, S.C. Smith, G.Q. Lu, H.G. Yang, "Higher Charge/Discharge Rates of Lithium-ions across Engineered TiO₂ Surfaces leads to Enhanced Battery Performance," *Chem. Comm.*, **46**, 6129-6131 (2010).
159. H. Zhang, Z.P. Xu, G. Q. Lu and S.C. Smith, "Computer Modelling Study for Intercalation of Drug Heparin into Layered Double Hydroxide," *J. Phys. Chem. C.*, **114**, 12618-12629 (2010).
157. G. Liu, C.H. Sun, S.C. Smith, L.Z. Wang, G.Q. Lu and H.M. Cheng "Sulfur Doped Anatase TiO₂ Single Crystals with a High Percentage of {001} Facets," *Journal of Colloid & Interface Science*, **349**, 477-483 (2010).
156. Y. Jiao, A. Du, Z. Zhu, V. Rudolph and S.C. Smith, "Adsorption of Carbon Dioxide and Nitrogen on Single Layer Aluminium Nitride Nanostructures Studied by Density Functional Theory," *J. Phys. Chem. C*, **114**, 7846-7849 (2010).
155. C. Sun, A. Du, G. Liu, S. Qiao, S.C. Smith and G.Q. Lu, "Formation Energies of Low-indexed Surfaces of Tin Dioxide Terminated by Nonmetals" *Solid State Commun.*, **150**, 957-960 (2010).
151. A.J. Du, Z.H. Zhu and S.C. Smith, "Multifunctional Porous Graphene for Nanoelectronics and Hydrogen Storage: New Properties Revealed by First Principle Calculations," *J. Amer. Chem. Soc.*, **132**, 2876-2877 (2010).
150. Z. Li, L. Cheng, Q. Sun, Z. Zhu, M.J. Riley, M. Aljada, Z. Cheng, X. Wang, S. Qiao, S.C. Smith and G.Q. Lu "Diluted Magnetic Semiconductor Nanowires Prepared by Solution-Liquid-Solid Method," *Angew. Chem. Int. Ed.*, **122**, 2837-2841 (2010).
149. Y. Wang, C.H. Sun, J. Zou, L.Z. Wang, S.C. Smith, G.Q. Lu and D.J.H. Cockayne, "Oxygen Vacancy induced Structural Variations of Exfoliated Monolayer MnO₂ Sheets," *Phys. Rev. B. rapid communication*, **81**, 081401 (4 pages) (2010).
146. G. Liu, C. Sun, H.G. Yang, S.C. Smith, G.Q. Lu and H.M. Cheng "Nanosized Anatase TiO₂ Single Crystals for Enhanced Photocatalytic Activity," *Chem. Comm.*, **46**, 755-757 (2010).
144. A.J. Du, Y. Chen, Z.H. Zhu, R. Amal, G.Q. Lu, S.C. Smith, "Dots versus Antidots: Computational Exploration of Structure, Magnetism and Half-metallicity in Boron-Nitride Nanostructures," *J. Amer. Chem. Soc.*, **131**, 17354-17359 (2009).
140. A.J. Du, C.H. Sun, G.Q. Lu, V. Rudolph, Z.H. Zhu, S.C. Smith, "The Effect of Fe Doping on Adsorption of CO₂/N₂ within Carbon Nanotubes: A Density Functional Theory Study with Dispersion Corrections," *Nanotechnology*, **20**,375701 (2009).
137. G. Liu, C.H. Sun, L. Cheng, Y.G. Jin, H.F. Lua, L.Z. Wang, S.C. Smith, G.Q. Lu, H.M. Cheng, "Efficient Promotion of Anatase TiO₂ Photocatalysis via Bifunctional Surface-Terminating Ti-O-B-N Structures," *J. Phys. Chem. C.*, **113**, 12317-12324 (2009).
134. G. Liu, C.H. Sun, X.X. Yan, L. Cheng, Z.G. Chen, X.W. Wang, L.Z. Wang, S.C. Smith, G.Q. Lu and H.M. Cheng, "Iodine Doped Anatase TiO₂ Photocatalyst with Ultra-long Visible Light Response: Correlation between Geometric/Electronic Structures and Mechanisms," *J. Mater. Chem.*, **19**, 2822-2829 (2009).
133. G. Liu, L.Z. Wang, C.H. Sun, X.X. Yan, X.W. Wang, Z.G. Chen, S.C. Smith, H.M. Cheng, G.Q. Lu, "Band-to-Band Visible-Light Photon Excitation and Photoactivity Induced by Homogeneous Nitrogen Doping in Layered Titanates," *Chem. Mat.*, **21**, 1266-1274 (2009).

132. H.G. Yang, G. Liu, S.Z. Qiao, C.H. Sun, Y.G. Jin, S.C. Smith, J. Zou, H.M. Cheng, G.Q. Lu, "Solvochemical Synthesis and Photoreactivity of Anatase TiO₂ Nanosheets with Dominant {001} Facets," *J. Amer. Chem. Soc.*, **131**, 4078-4083 (2009).
131. A.J. Du, Y. Chen, Z.H. Zhu, G.Q. Lu and S.C. Smith, "C-BN Single Walled Nanotubes from Hybrid Connection of BN/C Nanoribbons: Prediction by Ab Initio Density Functional Calculations," *J. Amer. Chem. Soc., rapid communication*, **131**, 1682-1683 (2009).
130. A.J. Du, Y. Chen, Z.H. Zhu, G.Q. Lu and S.C. Smith, "First Principle Studies of Zigzag AlN Nanoribbon," *Chem. Phys. Lett.*, **469**, 183-185 (2009).
129. A.J. Du, Z.H. Zhu, C.H. Sun, Y. Chen, G.Q. Lu, S.C. Smith, "Half Metallicity in a Zigzag Double Walled Nanotube Nanodot: an *ab initio* Prediction," *Chem. Phys. Lett.*, **468**, 257-259 (2009).
127. H. Zhang, Z.P. Xu, G.Q. Lu and S.C. Smith, "Intercalation of Sulfonate into Layered Double Hydroxide: Comparison of Simulation with Experiment," *J. Phys. Chem. C*, **113**, 559-566 (2009).
125. L. Li, X.D. Yao, C.H. Sun, A.J. Du, L. Cheng, Z.H. Zhu, C.Z. Yu, J. Zou, S.C. Smith, P. Wang, H.M. Cheng, R.L. Frost and G.Q. Lu, "Lithium-Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage," *Advanced Functional Materials*, **19**, 265-271 (2009).
- *124. A.J. Du, S.C. Smith, C.H. Sun, L. Li, X.D. Yao and G.Q. Lu, "First Principle Study of Hydrogenation of MgB₂: An Important Step toward Reversible Hydrogen Storage in the Coupled LiBH₄/MgH₂ System," *J. Nanosci. Nanotech.*, **9**, 4388-4391 (2009).
122. A. Du, S. C. Smith, X. D. Yao, C. H. Sun, L. Li and G.Q. Lu, "The Role of V₂O₅ on the Dehydrogenation and Hydrogenation in Magnesium Hydride: an *ab initio* Study," *Applied Physics Letters*, **92**, 163106 (3 pages) (2008).
119. C.H. Sun, X.D. Yao, A.J. Du, L. Li, S.C. Smith, G.Q. Lu, "Computational Study of Methyl Derivatives of Ammonia Borane for Hydrogen Storage," *Phys. Chem. Chem. Phys.*, **10**, 6104-6106 (2008).
118. A.J. Du, Y. Chen, G.Q. Lu and S.C. Smith, "Anti-ferromagnetism and Half-Metallicity in Finite-length Single Walled Zigzag Carbon Nanotubes as Predicted by *ab initio* Density Functional Calculations," *Applied Physics Letters*, **93**, 073101 (3 pages) (2008) [article featured on front cover].
117. H.G. Yang, C.H. Sun, S.Z. Qiao, J. Zhou, S.C. Smith, H.M. Cheng and G.Q. Lu, "Anatase TiO₂ Single Crystals with a Large Percentage of {001} Facets," *Nature*, **453**, 638-641 (2008).
113. P. Tran, H. Zhang, S.C. Smith, Y. Wong, Z.P. Xu and G.Q. Lu, "Molecular Dynamic Simulations of Interactions between LDH and NO₃⁻ intercalates in Aqueous Solution.," *J. Phys. Chem. Solid.*, **69**, 1044-1047 (2008).
- *111. A.J. Du, Sean C. Smith and G.Q. Lu, "Surface Interactions of a Ti Atom with Sodium Alanate: an *ab initio* Spin-polarized Study," (invited paper for the 2006 Australia - Brazil Bio Nanotechnology Conference) *Int. J. Nanotech.*, **4**, 564-573 (2007).
110. A. Du, S.C. Smith and G.Q. Lu, "Formation of Single Walled Carbon Nanotube Via the Interaction of Graphene Nanoribbons: *ab initio* Density Functional Calculations," *Nano Lett.*, **7**, 3349-3354 (2007).
109. A. Du, S.C. Smith and G.Q. Lu, "First Principle Studies of Electronic Structure and C-doping effect in Boron Nitride Nanoribbon," *Chem. Phys. Lett.*, **447**, 181-186 (2007) [selected as "Editor's Choice" article featured on front cover].
107. X. Yao, C.Z. Wu, A.J. Du, J. Zou, Y. He, Z.H. Zhu, P. Wang, H.M. Cheng, S.C. Smith, G.Q. Lu, "Metallic and Carbon Nanotube-Catalyzed Coupling of Hydrogenation in Magnesium," *J. Amer. Chem. Soc.*, **129**, 15650-15654 (2007).

106. A. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "Hydrogen Spillover Mechanism on a Pd-doped Mg Surface as Revealed by *ab initio* Density Functional Calculations," *J. Amer. Chem. Soc.*, **129**, 10201-10204 (2007).
105. A. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "The Role of Lithium Vacancies in Accelerating the Dehydrogenation Kinetics on a LiBH₄(010) Surface: an *ab initio* Study," *J. Phys. Chem. C*, **111**, 12124-12128 (2007).
104. A. Du, S.C. Smith and G.Q. Lu, "The Catalytic Role of Ti in the Dissociation of H₂ on a Ti-doped Al(001) Surface: an *ab initio* Density Functional Calculation," *Chem. Phys. Lett.*, **450**, 80-85 (2007).
103. B.Wanno, A.J.Du, V. Ruangpornvisuti, S.C. Smith, "Addition of Diazomethane to Armchair Single-walled Carbon Nanotubes and their Reaction Sequences: A Theoretical Prediction," *Chem. Phys. Lett.*, **436**, 218 – 223 (2007).
99. A.J. Du, Sean C. Smith and G.Q. Lu, "Vacancy Assisted Desorption of Hydrogen from a Sodium Alanate Surface: an *ab initio* Study," *Appl. Phys. Lett.*, **90**, 143119 (3 pages) (2007).
97. A.J. Du, Sean C. Smith and G.Q. Lu, "First Principle Studies of the Formation and Diffusion of Hydrogen Vacancies in Magnesium Hydride," *J. Phys. Chem. C*, **111**, 8360-8365 (2007).
88. A. Du and Sean C. Smith, "Structural and Electronic Properties of Diazonium Functionalized (4, 4) Single Walled Carbon Nanotube: an *ab initio* Study," *Molecular Simulation*, **32**, 1213–1217 (2006).
87. A. Du, Sean C. Smith, X.D. Yao and G.Q. Lu, "First Principle Study of Adsorption of Hydrogen Molecules on Ti-doped Mg(0001) Surface," *J. Phys. Chem. B*, **110**, 21747 – 21750 (2006).
86. A.J. Du, G.Q. Lu and Sean C. Smith, "Role of Charge in Destabilizing AlH₄ and BH₄ Complex Anions for Hydrogen Storage Applications: *Ab initio* Density Functional Calculations," *Phys. Rev. B rapid communication*, **74**, 193405 (4 pages) (2006).
83. X. Yao, C.Z. Wu, A.J. Du, G.Q. Lu, H.M. Cheng, S.C. Smith, J. Zou and Y. He, "Mg-based Nanocomposites with High Capacity and Fast Ad/desorption Kinetics for Hydrogen Storage," *J. Phys. Chem. B.*, **110**, 11697 - 11703 (2006).
82. A.J.Du, Sean C.Smith, X.D.Yao, Y. He and G.Q.Lu, "Atomic Hydrogen Diffusion in Novel Magnesium Nanostructures: The Impact of Incorporated Subsurface Carbon Atoms," Asian Consortium for Computational Materials Science Symposium proceedings, *Journal of Physics: Conference Series*, **29**, 167-172 (2006).
81. L.M. Kettle, H.S. Goan and S.C. Smith, "Molecular Orbital Calculations of Two-electron States for P Donor Solid-state Spin Qubits," *Phys. Rev. B*, **73**, 115205 (14 pages) (2006).
80. A.J. Du, S.C. Smith, X.D.Yao and G.Q. Lu, "*Ab initio* Studies of Hydrogen Desorption from Low Index Magnesium Hydride Surface," *Surf. Sci.*, **600**, 1854-1859 (2006).
78. A.J. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "Catalytic Effects of Sub-Surface Carbon in the Chemisorption of Hydrogen on a Mg(0001) Surface: an *Ab-Initio* Study," *J. Phys. Chem. B*, **110**, 1814-1819 (2006).
77. A.J. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "The Role of Ti as a Catalyst for the Dissociation of H₂ on a Mg(0001) Surface," *J. Phys. Chem. B*, **109**, 18037-18041 (2005).
75. A.J. Du and S.C. Smith, "Van der Waals-corrected Density Functional Theory: Benchmarking for Hydrogen-Nanotube and Nanotube-Nanotube Interactions," *Nanotechnology*, **16**, 2118-2123 (2005).
70. Z.H. Zhu, G.Q. Lu and S.C. Smith, "Comparative Study of Hydrogen Storage in Li- and K-doped Carbon materials - theoretically revisited," *Carbon*, **42**, 2509-2514 (2004).
64. L.M. Kettle, H.-S. Goan, Sean C. Smith, L.C.L. Hollenberg and C.J. Wellard, "Effects of *J*-Gate Potential and Interfaces on Donor Exchange Coupling in the Kane Quantum Computer Architecture," *J. Phys: Condens. Matter*

16, 1011-1023 (2004).

59. L.M. Kettle, H.S. Goan, S.C. Smith, L.C.L. Hollenberg, C.I. Pakes and C. Wellard, "A Numerical Study of Hydrogenic Effective Mass Theory for an Impurity P Donor in Si in the Presence of an Electric Field and Interfaces," *Phys. Rev. B*, **68**, 075317 (2003) (6 pages).

BIOMOLECULAR MODELLING

179. H. Sun, H-H Lee, I. Blakey, B. Dargaville, A.K. Whittaker and S.C. Smith, "Theoretical Study on 2-ureido-4[1H]-Pyrimidinone-based Multiple Hydrogen Bonded Complexes," *J. Phys. Chem. B* (accepted, August 2011).
177. D. Ouyang, H. Zhang, H.S. Parekh and S.C. Smith, "The Effect of pH on PAMAM Dendrimer-siRNA Complexation – Endosomal Considerations as Determined by Molecular Dynamics Simulation," *Biophys. Chem.* (accepted, June 2011).
161. Y.Y. Ma, Q. Sun, H. Zhang, L. Peng, J.G. Yu and S.C. Smith, "The Mechanism of Cyclization in Chromophore Maturation of Green Fluorescent Protein: A Theoretical Study," *J. Phys. Chem. B*, **114**, 9698-9705 (2010).
160. D. Ouyang, H. Zhang, D.-P. Herten, H.S. Parekh and S.C. Smith, "Structure and Dynamics of Multiple Cationic Vectors-siRNA Complexation by All-atomic Molecular Dynamics Simulations," *J. Phys. Chem. B*, **114**, 9231-9237 (2010).
158. D. Ouyang, H. Zhang, D.-P. Herten, H.S. Parekh and S.C. Smith, "Structure, Dynamics and Energetics of siRNA-Cationic Vector Complexation: A Molecular Dynamics Study," *J. Phys. Chem. B*, **114**, 9220-9230 (2010).
148. Q. Sun, M. Doerr, Z. Li, S.C. Smith and W. Thiel, "QM/MM Studies of Structural and Energetic Properties of the Far-red Fluorescent Protein HcRed," *Phys. Chem. Chem. Phys.*, **12**, 2450-2458 (2010).
147. Q. Sun, S. Wang, H. Zhang, Z. Li, C. Pfisterer, S. Fischer, S. Nanbu and S.C. Smith, "Structural and Relaxation Effects in Proton Wire Energetics: Model Studies of the Green Fluorescent Protein Photocycle," *Aust. J. Chem.*, **63**, 363-370 (2010).
139. H. Zhang, S. Wang, Q. Sun and S.C. Smith, "Kinetic Isotope Effect for Ground State Proton Transfer in the Green Fluorescent Protein: A Quantum-Kinetic Model," *Phys. Chem. Chem. Phys.*, **11**, 8422-8424 (2009) (selected as PCCP "hot article").
138. D. Ouyang, H. Zhang, D.P. Herten, H.S. Parekh and S.C. Smith, "Flexibility of Short-Strand RNA in Aqueous Solution as Revealed by Molecular Dynamics Simulation: Are A-RNA and A'-RNA Distinct Conformational Structures?" *Aust. J. Chem.*, **62**, 1054-1061 (2009).
135. D. Ouyang, N. Shah, H. Zhang, S.C. Smith and H. Parekh, "Reducible Disulphide-Based Non-Viral Gene Delivery Systems," *Mini Reviews in Medicinal Chemistry*, **9**, 1242-1250 (2009).
116. S. Olsen and S.C. Smith, "Bond Selectivity in the Photoisomerisation Reactions of Model GFP and KFP Chromophore Anions," *J. Amer. Chem. Soc.*, **130**, 8677-8689 (2008).
115. S.P. Nighswander-Rempel, S. Olsen, I.B. Mahadevan, G. Natchev, B.C. Wilson, S.C. Smith, H. Rubinsztein-Dunlop and Paul Meredith, "Effect of Dimerisation on Vibrational Spectra of Melanin Pre-cursors," *Photochem. Photobiol.*, **84**, 613-619 (2008).
108. H. Zhang and S.C. Smith, "Model Real-Time Quantum Dynamical Simulations of Proton Transfer in the Green Fluorescent Protein (GFP)," *J. Theor. Comput. Chem.*, **6**, 789-802 (2007).

102. S. Olsen, J. Riesz, I. Mahadevan, A. Coutts, B.J. Powell, R.H. McKenzie, S.C. Smith and P. Meredith, "Convergent Proton Transfer Photocycles Violate Mirror-Image Symmetry in a Key Melanin Monomer," *J. Amer. Chem. Soc. rapid communication*, **129**, 6672-6673 (2007).
100. J. Battad, P.G. Wilmann, S. Olsen, E. Byres, S.C. Smith, K. Turcic, R.J. Devenish, J. Rossjohn and M. Prescott "The Structural Basis for Increased Fluorescence Efficiency of the Chromoprotein Rtms5 at High pH," *J. Molec. Biol.*, **368**, 998 – 1010 (2007).
98. S. Wang and Sean C. Smith, "Mechanistic Aspects of Proton Chain Transfer in the Green Fluorescent Protein. II: A Comparison of Minimal Quantum Chemical Models," *Phys. Chem. Chem. Phys.*, **9**, 452-458 (2007) (front cover feature, Issue 4, 2007).
96. Seth Olsen and Sean C. Smith, "Radiationless Decay of Red Fluorescent Protein Chromophore Models via Twisted Intramolecular Charge-Transfer States," *J. Amer. Chem. Soc.*, **129**, 2054 – 2065 (2007).
- *91. S. Wang and S.C. Smith, "Leading Coordinate Analysis of Reaction Pathways in Proton Chain Transfer: Application to a Two-proton Transfer Model for the Green Fluorescent Protein," *Chem. Phys.*, (invited contribution to special edition in honour of 80th birthday of Professor Noel Hush), **326**, 204-209 (2006).
- *90. P. Wilmann, J. Battad, T. Beddoe, S. Olsen, S. Smith, S. Dove, R. Devenish, J. Rossjohn and M. Prescott, "The 2.0Å Crystal Structure of a Pociilloporin at pH 3.5: The Structural Basis for the Linkage of Colour Transition to Binding of Halides," *Photochemistry and Photobiology*, **82**, 359-366 (2006).
85. Seth Olsen and Sean C. Smith, "Trans-Cis Isomerism and Acylimine Formation in DsRed Chromophore Models: Intrinsic Rotation Barriers," *Chem. Phys. Lett.*, **426**, 159-162 (2006).
84. S.C. Olsen, M. Prescott, P. Wilmann, J. Battad, J. Rossjohn and Sean C. Smith "Determination of Chromophore Charge States in the Low pH Color Transition of the Fluorescent Protein Rtms5H146S via Time-Dependent DFT," *Chem. Phys. Lett.*, **420**, 507-511 (2006).
79. S. Wang and S.C. Smith, "Mechanistic Aspects of Proton Chain Transfer: A Computational Study for the Green Fluorescent Protein Chromophore," *J. Phys. Chem. B.*, **110**, 5084-5093 (2006).
74. P.G. Wilmann, J. Petersen, A.Z. Pettikiriachchi, A.M. Buckle, S.C. Smith, S. Olsen, M.A. Perugini, R.J. Devenish, M. Prescott and J. Rossjohn, "The 2.1 Å Crystal Structure of the Far-red Fluorescent Protein HcRed: Inherent Conformational Flexibility of the Chromophore.," *J. Molecular Bio.*, **349**, 223-237 (2005).

GAS PHASE QUANTUM DYNAMICS

168. H. Yang, K.-L. Han, G.C. Schatz, S.C. Smith and M. Hankel, "Exact and Truncated Coriolis Coupling Calculations for the S(¹D)+HD Reaction Employing the Ground Adiabatic Electronic State," *Phys. Chem. Chem. Phys.*, **12**, 12711-12718 (2010).
154. S. Olsen, D. Schwarzer, J. Troe and S.C. Smith, "Quantum Chemical Characterization of Low-Lying Excited States of an Arylperoxycarbonate: Mechanistic Implications for Photodissociation," *J. Phys. Chem. A*, **114**, 4289-4295 (2010).
153. H. Zhang, S.C. Smith, S. Nanbu and H. Nakamura, "First Principle Study of Atomic Hydrogen Interaction with Fluorinated Corannulene Radical," *Aust. J. Chem.*, **63**, 371-378 (2010).
143. P.G. Jambrina, F.J. Aoiz, N. Bulut, S.C. Smith, G.G. Balint-Kurti and M. Hankel, "The Dynamics of the H⁺+D₂ Reaction: A Comparison of Quantum Mechanical Wavepacket, Quasi-classical and Statistical-quasi-Classical Results," *Phys. Chem. Chem. Phys.*, **12**, 1102-1115 (2010).

142. H. Yang, K.-L. Han, G. C. Schatz, S. C. Smith, M. Hankel, "Quantum Mechanical Calculations of the S(1D)+HD Reaction Dynamics on the Ground Electronic State," *J. Phys.: Conf. Ser.*, **185**, 012056 (4 pages) (2009).
141. H. Yang, K.-L. Han, G. C. Schatz, S. H. Lee, K. Liu, S. C. Smith and M. Hankel, "Integral and Differential Cross Sections for the S(1D)+HD Reaction Employing the Ground Adiabatic Electronic State," *Phys. Chem. Chem. Phys.*, **11**, 11587-11595 (2009).
128. H. Yang, K. Han, S. Nanbu, H. Nakamura, G.G. Balint-Kurti, H. Zhang, S.C. Smith and M. Hankel, "Boltzmann Averaged Branching Ratios and Vibrational Distributions for the O(¹D)+HCl → OH+Cl (OCl+H) Reaction," *J. Theor. Comp. Chem.*, **8**, 1003-1024 (2009).
126. H. Zhang, S.C. Smith, S. Nanbu and H. Nakamura, "Quantum Mechanical Study of Atomic Hydrogen Interaction with Fluorinated Boron-Substituted Coronene Radical," *J. Phys. Condens. Matt.*, **21**, 144209 (2009).
123. P. Bargueno, T. Gonzalez-Lazana, P. Larregaray, L. Bonnet, J.C. Rayez, M. Hankel, S.C. Smith and A.J.H.M. Meijer, "Study of the H+O₂ Reaction by Means of Quantum Mechanical and Statistical Approaches: The Dynamics on Two Different Potential Energy Surfaces," *J. Chem. Phys.*, **128**, 244308 (14 pages) (2008).
121. H. Yang, K.L. Han, S. Nanbu, H. Nakamura, G.G. Balint-Kurti, H. Zhang, S.C. Smith and M. Hankel, "Energy Dependence of Branching Ratios and Product State Distributions for the O(¹D)+HCl Reaction," *J. Phys. Chem. A*, **112**, 7947-7960 (2008).
120. H. Zhang, M. Hankel, S. Nanbu, H. Nakamura and S.C. Smith, "Quantum Calculation of Ro-vibrational States: Methodology and DOCl Application Results," *J. Phys Chem A*, **112**, 4141-4147 (2008).
114. M. Hankel, S.C. Smith, S.K. Gray and G.G. Balint-Kurti, "DIFFREALWAVE: A Parallel Real Wavepacket Code for the Quantum Mechanical Calculation of Reactive State-to-state Differential Cross Sections in Atom plus Diatom Collisions," *Comput. Phys. Commun.*, **179**, 569-578 (2008).
112. H. Yang, K.-L. Han, S. Nanbu, H. Nakamura, G.G. Balint-Kurti, H. Zhang, S.C. Smith and M. Hankel, "Quantum Dynamics Study of the O(¹D)+HCl Reaction Employing Three Electronic States," *J. Chem. Phys.*, **128**, 014308 (5 pages) (2008).
101. M. Hankel, S.C. Smith and A.J.H.M. Meijer, "State-to-State Reaction Probabilities for the H+O₂(*v*, *j*) → O+OH(*v'*, *j'*) Reaction on Three Potential Energy Surfaces," *J. Chem. Phys.*, **127** 064316 (10 pages) (2007).
- *93. H. Zhang, S.C. Smith, S. Nanbu and H. Nakamura, "HOCl Ro-vibrational Bound State Calculations for Non-Zero Total Angular Momentum," *J. Phys. Chem. A*, **110**, 5468-5474 (2006) (invited contribution to the special edition in honour of Prof. J.C. Light's 65th birthday).
- *92. H. Zhang and S.C. Smith, "HO₂ Ro-vibrational State Calculations for Large Angular Momentum: *J* = 30, 40, and 50," *J. Phys. Chem. A*, **110**, 3246-3253 (2006) (invited contribution to special edition in honour of Professor Jürgen Troe's 65th birthday).
89. Marlies Hankel, Sean C. Smith, Robert J. Allan, Stephen K. Gray and Gabriel G. Balint-Kurti, "State-to-state Reactive Differential Cross Sections for the H + H₂ → H₂ + H Reaction on Five Different Potential Energy Surfaces Employing a New Quantum Wavepacket Computer Code; DiffRealWave.," *J. Chem. Phys.*, **125**, 164303 (2006) (12 pages).
76. H. Zhang and S.C. Smith, "Unimolecular Ro-vibrational Bound and Resonance States for Large Angular Momentum: *J* = 20 Calculations for HO₂," *J. Chem. Phys.*, **123**, 014308 (9 pages) (2005).
- *73. H. Zhang and S.C. Smith, "Symmetry Contaminations in Reactive Scattering through Long-Lived Collision Complexes," *Chem. Phys.*, **308**, 297-304 (2005) (special memorial edition in honour of Gert du Billing).
68. A.J. Rasmussen and Sean C. Smith, "A Lanczos-Powered Implementation of the Faber Polynomial Quantum

- Time Propagator for Reaction Probabilities,” *Chem. Phys. Lett.*, **387**, 277-282 (2004).
67. H. Zhang and S.C. Smith, “Converged Quantum Calculations of HO₂ Bound States and Resonances for $J = 6$ and 10,” *J. Chem. Phys.*, **120**, 9583-9593 (2004).
 66. H. Zhang and S.C. Smith, “Iterative Quantum Computations of HO₂ Bound States and Resonances for $J = 4$ and 5,” *Phys. Chem. Chem. Phys.*, **6**, 4240-4246 (2004).
 65. H. Zhang and S.C. Smith, “Full S Matrix Calculation via a Single Real-Symmetric Lanczos Recursion: The Lanczos ABI Method,” *J. Chem. Phys. (rapid communication)*, **120**, 1161-1163 (2004).
 - *63. Hong Zhang and Sean C. Smith, “A Comparative Study of Iterative Chebyshev and Lanczos Implementations of the Boundary Inhomogeneity Method for Quantum Scattering,” *J. Theor. Comput. Chem.* **2**, 563-572 (2003) (refereed manuscript in association with invited presentation at ACS symposium on iterative methods in quantum dynamics, New Orleans, March 2003).
 60. H. Zhang and S.C. Smith, “Calculation of Bound and Resonance States of HO₂ for Non-Zero Total Angular Momentum,” *J. Chem. Phys.*, **118**, 10042-10050 (2003).
 57. D. Reignier and S.C. Smith, “A Real Symmetric Lanczos Subspace Implementation of Quantum Scattering using Boundary Inhomogeneities,” *Chem. Phys. Lett.*, **366**, 390-397 (2002).
 56. H. Zhang and S.C. Smith, “Chebychev Real Wave Packet Propagation: H + O₂ ($J = 0$) State-to-State Reactive Scattering Calculations,” *J. Chem. Phys.*, **117**, 5174-5182 (2002).
 54. H. Zhang and S.C. Smith, “Lanczos Subspace Time-Independent Wavepacket Calculations of S (¹D) + H₂ Reactive Scattering,” *J. Phys. Chem. A*, **106**, 6137-6142 (2002).
 53. H. Zhang and S.C. Smith, “Calculation of Resonances and Product State Distributions for the Unimolecular Dissociation of H₂S,” *J. Phys. Chem. A*, **106**, 6129-6136 (2002).
 52. H. Zhang and S.C. Smith, “Efficient Time-Independent Wavepacket Scattering Calculations within a Lanczos Subspace: H+O₂ ($J=0$) State-to-State Reaction Probabilities,” *J. Chem. Phys.* **116**, 2354-2360 (2002).
 49. H. Zhang and S.C. Smith, “Calculation of Product State Distributions from Resonance Decay via Lanczos Subspace Filter Diagonalization: Application to HO₂,” *J. Chem. Phys.* **115**, 5751-5758 (2001).
 47. H. Zhang and S.C. Smith, “A Comparison of Low-Storage Strategies for Spectral Analysis in Dissipative Systems: Filter Diagonalization in the Lanczos Representation and Harmonic Inversion of the Chebychev-Order-Domain Autocorrelation Function,” *Chem. Phys. Lett.*, **347**, 211-219 (2001).
 46. H. Zhang and S.C. Smith, “Lanczos Subspace Filter Diagonalization: Homogeneous Recursive Filtering and a Low-Storage Method for the Calculation of Matrix Elements,” *Phys. Chem. Chem. Phys.*, **3**, 2282 - 2288 (2001).
 45. A.J. Rasmussen, S.J. Jeffrey and S.C. Smith, “Subspace Wavepacket Evolution with Newton Polynomials,” *Chem. Phys. Lett.*, **336**, 149-155 (2001).
 41. J.T. Lin, J.M. Yuan, S.C. Smith and S.H. Lin, “Dissociation Dynamics of HeRh²⁺ in Field-Ion Microscopy,” *Phys. Rev. B*, **61**, 9419-9426 (2000).
 - *40. S.C. Smith, H.-G. Yu, C. Leforestier and J.-C. Rayez, “Optimal Spectral Filtering in a Finite Subspace: a Lanczos-Based Implementation,” *Phys. Chem. Chem. Phys.*, **1** (Special Issue on Chemical Reaction Theory, ed. J.N.L. Connor), 1311-1316 (1999).
 39. A.J. Rasmussen and S.C. Smith, “Circulants, Symmetry and Time-Independent Wavepacket Scattering,” *Chem. Phys. Lett.*, **312**, 229-236 (1999).

37. A.J. Rasmussen, K.E. Gates and S.C. Smith, "A pseudo-Spectral Algorithm for the Computation of Transitional-Mode Eigenfunctions in Loose Transition States. II. Optimized Primary and Grid Representations," *J. Chem. Phys.*, **110**, 1354-1364 (1999).
36. V. Szalay and S.C. Smith, "Application of Contracted Distributed Approximating Functions to Solving Vibrational Eigenvalue Problems," *J. Chem. Phys.*, **110**, 72-79 (1999).
34. H.G. Yu and S.C. Smith, "Calculation of Quantum Resonance Energies and Lifetimes via Quasi-Minimum Residual Filter Diagonalization," *Chem. Phys. Lett.* **283**, 69-76 (1998).
33. H.G. Yu and S.C. Smith, "The Elimination of Lanczos Ghosting by MINRES Filter Diagonalization," *J. Comp. Phys.* **143**, 484-494 (1998).
- *32. H.G. Yu and S.C. Smith, "The Calculation of Vibrational Eigenstates by MINRES Filter Diagonalization," *Ber. Bunsenges. Phys. Chem.* **101**, 400-406 (1997).
- *31. H.G. Yu and S.C. Smith, "Restarted Krylov-Space Spectral Filtering," *Faraday Transactions*, **93** (Special Issue on Theory of Chemical Reactions, ed. D.C. Clary), 861-869 (1997).
30. S.J. Jeffrey and S.C. Smith, "Calculation of Absolute Spectral Densities via Stochastic Trace Estimators of $\text{tr}\{\delta(E-H)\}$," *Chem. Phys. Lett.* **278**, 345-351 (1997).
29. H.G. Yu and S.C. Smith, "The Simulation of Outgoing-Wave Boundary Conditions via a Symmetrically-Damped Hermitian Hamiltonian Operator," *J. Chem. Phys.* **107**, 9985-9993 (1997).
26. S.J. Jeffrey, S.C. Smith and D.C. Clary, "Calculation of the Vibrational Spectral Density of NO₂ via Density Correlation Functions," *Chem. Phys. Lett.* **273**, 55-61 (1997).
- *23. S.C. Smith, "Towards Quantum Mechanical Characterization of the Dissociation Dynamics of Ketene," *Faraday Discussion* **102**, 17-29 (1996).
21. S.C. Smith and S.J. Jeffrey, "On the Calculation of Absolute Spectral Densities," *J. Chem. Phys.* **105**, 4055-4064 (1996).
19. S.C. Smith, "A Pseudo-Spectral Algorithm for the Computation of Transitional Mode Eigenfunctions in Loose Transition States," *Chem. Phys. Lett.* **243**, 359-366 (1995).

STATISTICAL THEORIES AND CHEMICAL KINETICS

152. H. Zhang and S.C. Smith, "Calculation of HO₂ Density of States on Three Potential Energy Surfaces," *J. Theor. Comp. Chem.*, accepted (Feb 2010).
145. Craig A. Bell, Qiao Sun, Hong Zhang, Sean C. Smith, Paul V. Bernhardt, Michael J. Monteiro, "Methyl Acrylate Polymerizations in the Presence of a Copper/N₃S₃ Macrobicyclic Cage in DMSO at 25 °C," *Polymer Chemistry*, **1**, 207-212 (2010).
- *136. T.J. Frankcombe and S.C. Smith, "Numerical Solution Methods for Large, Difficult Kinetic Master Equations," *Theor. Chem. Act.*, **124**, 303-317 (2009).
- *95. T.J. Frankcombe and S.C. Smith, "OH-initiated Oxidation of Toluene. II. Master Equation Simulation of Toluene Oxide Isomerisation," *J. Phys. Chem. A*, **111**, 3691-3696 (2007). (invited contribution to the special edition in honour of J. Miller's 60th birthday).
- *94. T.J. Frankcombe and S.C. Smith, "OH-initiated Oxidation of Toluene. I. Quantum Chemistry Investigation of the Reaction Path," *J. Phys. Chem. A*, **111**, 3686 – 3690 (2007). (invited contribution to the special edition in honour

of J. Miller's 60th birthday).

72. A.C. Olleta, S.I. Lane and S.C. Smith, "Transition-State-Theory Calculations for Reactions of O(³P) with Halogenated Olefins," *Phys. Chem. Chem. Phys.*, **6**, 5362-5369 (2004).
71. T.J. Frankcombe and S.C. Smith, "On the Mechanism of Carbon Gasification: A Theoretical Study," *Carbon*, **42**, 2921-2928 (2004).
69. V.V. Kislov, T.L. Nguyen, S.H. Lin, A.M. Mebel and S.C. Smith, "Photodissociation of Benzene under Collision-free Conditions: An Ab Initio/RRKM Study," *J. Chem. Phys.*, **120**, 7008-7017 (2004).
62. T.J. Frankcombe and S.C. Smith, "Fast, Scalable Master Equation Solution Algorithms. IV. Lanczos Iteration with Diffusion Approximation Preconditioned Iterative Inversion," *J. Chem. Phys.* **119**, 12741-12748 (2003).
61. T.J. Frankcombe and S.C. Smith, "Fast, Scalable Master Equation Solution Algorithms. III: Direct Time Propagation Accelerated by a Diffusion Approximation Preconditioned Iterative Solver," *J. Chem. Phys.* **119**, 12729-12740 (2003).
58. T.J. Frankcombe and S.C. Smith, "Selecting Methods for Solving Multi-well Master Equations," *J. Theor. Comput. Chem.*, **2**, 179-191 (2003).
55. H.W. Schranz, S.C. Smith, A.M. Mebel, and S.H. Lin "Prediction of Absolute Rate Coefficients and Product Branching Ratios for the C(³P) + Allene Reaction System," *J. Chem. Phys.* **117**, 7055-7067 (2002).
51. T. J. Frankcombe, S. Bhatia and S.C. Smith, "Ab Initio Modelling of Basal Plane Oxidation of Graphenes and Implications for Modelling Char Combustion," *Carbon*, **40**, 2341-2349 (2002).
- *50. T.J. Frankcombe, S.C. Smith, "Time-Dependent Master Equation Simulation of Complex Elementary Reactions in Combustion: Application to the Reaction of ¹CH₂ with C₂H₂ from 300-2000K." *Faraday Discussion* **119**, 159-171 (2001).
48. T.J. Frankcombe and S.C. Smith, "Time Evolution in the Unimolecular Master Equation at Low Temperatures: Full Spectral Solution with Scalable Iterative Methods and High Precision," *Comput. Phys. Comm.* **141**, 39-54 (2001).
- *44. T.J. Frankcombe, S.C. Smith, K.E. Gates and S.H. Robertson, "A Master Equation Model for Bimolecular Reaction via Multi-well Isomerising Intermediates," *Phys. Chem. Chem. Phys.*, **2** (Special Issue on Molecular Reaction Dynamics: Experiment and Theory, ed. J.N.L. Connor), 793-803 (2000).
43. S.C. Smith, "Kinematic Factors in Transition State Theory with a Generalized Reaction Coordinate," *J. Phys. Chem. A*, **104**, 10489-10499 (2000).
42. T.J. Frankcombe and S.C. Smith, "Solving the Unimolecular Master Equation with a Weighted Subspace Projection Method," *J. Comput. Chem.*, **21**, 592-606 (2000).
38. S.C. Smith, "Classical Flux Integrals in Transition State Theory: Generalized Reaction Coordinates," *J. Chem. Phys.*, **111**, 1830-1842 (1999).
35. N. Marchand, J.C. Rayez and S.C. Smith, "Theoretical Study of the Reaction CH(X²Π) + NO(X²Π). III. Determination of the Branching Ratios," *J. Phys. Chem. A* **102**, 3358 -3367 (1998).
28. S.C. Smith, M.J. McEwan and J.I. Brauman, "The Reversibility Relationship in Collision-Complex-Forming Bimolecular Reactions," *J. Phys. Chem. A*, **101**, 7311-7314 (1997).
27. K.E. Gates, S.H. Robertson, K. Maschoff, S.C. Smith, M. Beazley and M.J. Pilling, "Multiple-Well Isomerization Diffusion Equation Solutions with a Shift-and-Invert Lanczos Algorithm," *J. Phys. Chem. A* **101**, 5765-5769

(1997).

25. S.H. Robertson, M.J. Pilling, K.E. Gates and S.C. Smith, "Application of Inverse Iteration to 2-Dimensional Master Equations," *J. Comput. Chem.* **18**, 1004-1010 (1997).
24. E. W.-G. Diau and S.C. Smith, "Theoretical Investigation of the Potential Energy Surface for the NH_2+NO Reaction via Density Functional Theory and Ab Initio Molecular Electronic Structure Theory," *J. Chem. Phys.* **106**, 9236-9251 (1997).
22. E. W.-G. Diau and S.C. Smith, "Temperature Dependence of Rate Coefficients and Branching Ratios for the NH_2+NO Reaction via Microcanonical Variational Transition State Theory," *J. Phys. Chem.* **100**, 12349-12354 (1996).
20. S. Jeffrey, K.E. Gates and S.C. Smith, "Full Iterative Solution of the Two-Dimensional Master Equation for Thermal Unimolecular Reactions," *J. Phys. Chem.* **100**, 7090-7096 (1996).
18. Y. Guo, S.C. Smith, C.F. Melius and C.B. Moore, "Kinetics and Product Branching Ratios for the Reaction $\text{HCO} + \text{NO}_2$," *J. Phys. Chem.* **99**, 7473-7481 (1995).
17. V.G. Anicich, A.D. Sen, M.J. McEwan and S.C. Smith, "A Comparison of an Experimental Unimolecular Lifetime Distribution with RRKM Theory," *J. Chem. Phys.* **100**, 5696 (1994).
16. S.C. Smith, "Flux Factors in Variational Transition State Theory," *J. Phys. Chem.* **98**, 6496 (1994).
15. S.C. Smith, "Rapid Algorithms for Variational RRKM Theory," *J. Phys. Chem.* **97**, 7034 (1993).
14. S.C. Smith, P.F. Wilson, M.J. McEwan, P. Sudkeaw, R.G.A.R. Maclagan, W.T. Huntress, and V.G. Anicich, "Statistical Modeling of Capture, Association and Exit Channel Dynamics in the $\text{CH}_3^+/\text{CH}_3\text{CN}$ System," *J. Chem. Phys.* **98**, 1944 (1993).
13. S.C. Smith, "Angular-Momentum Resolution in Transitional-Mode State Counting for Loose Transition States," *J. Chem. Phys.* **97**, 2406 (1992).
12. S.C. Smith and J. Troe, "Statistical Modeling of Ion-Molecule Electrostatic Capture," *J. Chem. Phys.* **97**, 5451 (1992).
11. M.J.T. Jordan, S.C. Smith and R.G. Gilbert, "Variational Transition State Theory: A Simple Model for Dissociation and Recombination Reactions of Small Species," *J. Phys. Chem.* **95**, 8685 (1991).
10. S.C. Smith, "Microscopic Rate Coefficients in Reactions with Flexible Transition States: Analysis of the Transitional-Mode Sum of States," *J. Chem. Phys.* **95**, 3404 (1991).
9. M. Moet-Ner and S.C. Smith, "Entropy Barriers to Proton Transfer," *J. Amer. Chem. Soc.* **113**, 862 (1991).
8. S.C. Smith, M.J. McEwan, K. Giles, N.G. Adams and D. Smith, "Unimolecular Decomposition of a Polyatomic Ion in a Variable-Temperature Selected-Ion-Flow-Drift Tube: Experiment and Theoretical Interpretation," *Int. J. Mass. Spect. Ion. Proc.* **96**, 77 (1990).
7. S.C. Smith, M.J. McEwan and R.G. Gilbert, "Microscopic Reaction Rates in Ion-Molecule Reactions: Effects of Uncoupled Modes," *J. Phys. Chem.* **93**, 8142 (1989).
6. S.C. Smith, M.J. McEwan and R.G. Gilbert, "The Relationship between Recombination, Chemical Activation, and Unimolecular Dissociation Rate Coefficients," *J. Chem. Phys.* **90**, 4265 (1989).
5. S.C. Smith, M.J. McEwan and R.G. Gilbert, "The Pressure Dependence of Ion-Molecule Association Rate Coefficients," *J. Chem. Phys.* **90**, 1630 (1989).

4. S.C. Smith and R.G. Gilbert, "Program FALLOFF: Calculation of Falloff Curves for Unimolecular and Recombination Reactions through Solution of the Master Equation," *Quantum Chemistry Program Exchange* **8**, 168 (1988).
3. S.C. Smith and R.G. Gilbert, "Angular Momentum Conservation in Multichannel Unimolecular Reactions," *Int. J. Chem. Kinet.* **20**, 979 (1988).
2. S.C. Smith and R.G. Gilbert, "Angular Momentum Conservation in Unimolecular and Recombination Reactions," *Int. J. Chem. Kinet.* **20**, 307 (1988).
1. J.S. Knight, C.G. Freeman, M.J. McEwan, S.C. Smith, N.G. Adams and D. Smith, "Production and Loss of HC₃N in Interstellar Gas Clouds: Some Relevant Laboratory Measurements," *Mon. Not. R. Ast. Soc.* **219**, 89 (1986).

Refereed Journal Papers (Full Chronological Listing)

Invited papers marked with an asterisk.

Journals with impact factor above 4 are highlighted in blue.

180. C.H. Sun, A. Selloni, A. Du and S.C. Smith, "Interaction of Water with Fluorine-covered Anatase TiO₂ (001) Surface," *J. Phys. Chem. C* (accepted, August 2011).
179. H. Sun, H-H Lee, I. Blakey, B. Dargaville, A.K. Whittaker and S.C. Smith, "Theoretical Study on 2-ureido-4[1H]-Pyrimidinone-based Multiple Hydrogen Bonded Complexes," *J. Phys. Chem. B* (accepted, August 2011).
178. A. Mukherjia, C.H. Sun, S.C. Smith, G.Q. Lu and L.Z. Wang, "Photocatalytic Hydrogen Production from Water Using N-doped Ba₅Ta₄O₁₅ Under Solar Irradiation," *J. Phys. Chem. C* (accepted, June 2011).
177. D. Ouyang, H. Zhang, H.S. Parekh and S.C. Smith, "The Effect of pH on PAMAM Dendrimer-siRNA Complexation – Endosomal Considerations as Determined by Molecular Dynamics Simulation," *Biophys. Chem.* (accepted, June 2011).
176. Y. Jiao, A. Du, Z.H. Zhu, V. Rudolph, G.Q. Lu, S.C. Smith, "A Density Functional Theory Study on CO₂ Capture and Activation by Graphene-like Boron Nitride with Boron Vacancy," *Catalysis Today* (accepted, March 2011).
175. C.H. Sun, Y. Wang, J. Zou and S.C. Smith "A Formation Mechanism of Oxygen Vacancies in a MnO₂ Monolayer: A DFT + U Study," *Phys. Chem. Chem. Phys.*, (accepted, Apr 2011).
174. A. Du, Y.H. Ng, N. Bell, Z.H. Zhu, R. Amal and S.C. Smith, "Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole-doping and Sensitization for Visible Light Response," *J. Phys. Chem. Lett.*, (accepted, Mar 2011).
173. N. Bell, Y.H. Ng, A. Du, H. Coster, S.C. Smith and R. Amal, "Understanding the Enhancement in Photoelectrochemical Properties of Photocatalytically-prepared TiO₂-Reduced Graphene Oxide Composite," *J. Phys. Chem. C*, accepted (February, 2011).
172. M. Hankel, H. Zhang, T.X. Nguyen, S.K. Bhatia, S.K. Gray, and S.C. Smith, "Kinetic Modelling of Molecular Hydrogen Transport in Microporous Carbon Materials," *Phys. Chem. Chem. Phys.*, **13**, 7834-7844 (2011).
171. X. Zong, C.H. Sun, Z.G. Chen, A. Mukherji, R. Gilbert, H. Wu, J. Zou, S.C. Smith, G.Q. Lu and L.Z. Wang, "Nitrogen Doping In Ion-exchangeable Layered Tantalate towards Visible-light Induced Water Oxidation," *Chem. Comm.*, accepted (February, 2011).
170. C.H. Sun, A. Mukherji, G.Q. Liu, L. Wang and S.C. Smith, "Improved Visible Light Absorption of HTaWO₆ Induced by Nitrogen Doping: An Experimental and Theoretical Study," *Chem. Phys. Lett.*, **501**, 427-430 (2010).
169. R. Marschall, A. Mukherji, A. Tanksale, C.H. Sun, S.C. Smith, G.Q. Lu, L.Z. Wang, "Preparation of New Sulfur-doped and Sulfur/nitrogen Co-doped CsTaWO₆ Photocatalysts for Hydrogen Production from Water under Visible Light," *J. Mat. Chem.*, (accepted December 2010).
168. H. Yang, K.-L. Han, G.C. Schatz, S.C. Smith and M. Hankel, "Exact and Truncated Coriolis Coupling Calculations for the S(¹D)+HD Reaction Employing the Ground Adiabatic Electronic State," *Phys. Chem. Chem. Phys.*, **12**, 12711-12718 (2010).
167. Z. Li, X. Ma, Q. Sun, Z. Wang, J. Liu, Z.H. Zhu, S.Z. Qiao, S.C. Smith, G.Q. Lu and A. Mews, "Synthesis and Characterization of Colloidal Core-Shell Semiconductor Nanowires," *Eur. J. Inorg. Chem.*, **2010(27)**, 4325-4331(2010).

166. Y. Jiao, A. Du, Z. Zhu, V. Rudolph and S.C. Smith "A Density Functional Theory Study of CO₂ and N₂ Adsorption on Aluminium Nitride Single Walled Nanotubes," *J. Mat. Chem.*, **20**, 10426-10430 (2010).
165. A. Mukherji, R. Marschall, A. Tanksale, C.H. Sun, S.C. Smith, G.Q. Lu, L.Z. Wang, "N-doped CsTaWO₆ as a New Photocatalyst for Hydrogen Production from Water splitting under Solar Irradiation," *Adv. Funct. Mat.*, **21(1)**, 126-132(2010).
164. G. Liu, P. Niu, C.H. Sun, S.C. Smith, Z.G. Chen, G.Q. Lu and H.M. Cheng, "Unique Electronic Structure Induced High Photoreactivity of Sulfur-Doped Graphitic C₃N₄," *J. Amer. Chem. Soc.*, **132(33)**, 11642-11648, (2010).
163. C.H. Sun, X.H. Yang, J.S. Chen, Z. Li, X.W. Lou, C.Z. Li, S.C. Smith, G.Q. Lu, H.G. Yang, "Higher charge/discharge rates of lithium-ions across engineered TiO₂ surfaces leads to enhanced battery performance," *Chem. Comm.*, **46**, 6129-6131 (2010).
162. S.C. Smith and Q. Sun, "Molecular Modelling: All the way from Atomistic Structure to Function in Complex Systems," *Aust. J. Chem.*, **63**, 343-344 (2010).
161. Y.Y. Ma, Q. Sun, H. Zhang, L. Peng, J.G. Yu and S.C. Smith, "The Mechanism of Cyclization in Chromophore Maturation of Green Fluorescent Protein: A Theoretical Study," *J. Phys. Chem. B*, **114**, 9698-9705 (2010).
160. D. Ouyang, H. Zhang, D.-P. Herten, H.S. Parekh and S.C. Smith, "Structure and Dynamics of Multiple Cationic Vectors-siRNA Complexation by All-atomic Molecular Dynamics Simulations," *J. Phys. Chem. B*, **114**, 9231-9237(2010).
159. H. Zhang, Z.P. Xu, G.Q. Lu and S.C. Smith, "Computer Modelling Study for Intercalation of Drug Heparin into Layered Double Hydroxide," *J. Phys. Chem. C*, **114(29)**, 12618-12629 (2010).
158. D. Ouyang, H. Zhang, D.-P. Herten, H.S. Parekh and S.C. Smith, "Structure, Dynamics and Energetics of siRNA-Cationic Vector Complexation: A Molecular Dynamics Study," *J. Phys. Chem. B*, **114**, 9220-9230 (2010).
157. G. Liu, C.H. Sun, S.C. Smith, L.Z. Wang, G.Q. Lu and H.M. Cheng "Sulfur Doped Anatase TiO₂ Single Crystals with a High Percentage of {001} Facets," *Journal of Colloid & Interface Science*, **349**, 477-483 (2010).
156. Y. Jiao, A. Du, Z. Zhu, V. Rudolph and S.C. Smith, "Adsorption of Carbon Dioxide and Nitrogen on Single Layer Aluminium Nitride Nanostructures Studied by Density Functional Theory," *J. Phys. Chem. C*, **114**, 7846-7849 (2010).
155. C. Sun, A. Du, G. Liu, S. Qiao, S.C. Smith and G.Q. Lu, "Formation Energies of Low-indexed Surfaces of Tin Dioxide Terminated by Nonmetals" *Solid State Commun.*, **150**, 957-960 (2010).
154. S. Olsen, D. Schwarzer, J. Troe and S.C. Smith, "Quantum Chemical Characterization of Low-Lying Excited States of an Arylperoxycarbonate: Mechanistic Implications for Photodissociation," *J. Phys. Chem. A*, **114**, 4289-4295 (2010).
153. H. Zhang, S.C. Smith, S. Nanbu and H. Nakamura, "First Principle Study of Atomic Hydrogen Interaction with Fluorinated Corannulene Radical," *Aust. J. Chem.*, **63**, 371-378 (2010).
152. H. Zhang and S.C. Smith, "Calculation of HO₂ Density of States on Three Potential Energy Surfaces," *J. Theor. Comp. Chem.*, accepted (Feb 2010).
151. A.J. Du, Z.H. Zhu and S.C. Smith, "Multifunctional Porous Graphene for Nanoelectronics and Hydrogen Storage: New Properties Revealed by First Principle Calculations," *J. Amer. Chem. Soc.*, **132**, 2876-2877 (2010).

150. Z. Li, L. Cheng, Q. Sun, Z. Zhu, M.J. Riley, M. Aljada, Z. Cheng, X. Wang, S. Qiao, S.C. Smith and G.Q. Lu "Diluted Magnetic Semiconductor Nanowires Prepared by Solution-Liquid-Solid Method," *Angew. Chem. Int. Ed.*, **122**, 2837-2841 (2010).
149. Y. Wang, C.H. Sun, J. Zou, L.Z. Wang, S.C. Smith, G.Q. Lu and D.J.H. Cockayne, "Oxygen Vacancy Induced Structural Variations of Exfoliated Monolayer MnO₂ Sheets," *Phys. Rev. B. rapid communication*, **81**, 081401 (4 pages) (2010).
148. Q. Sun, M. Doerr, Z. Li, S.C. Smith and W. Thiel, "QM/MM Studies of Structural and Energetic Properties of the Far-red Fluorescent Protein HcRed," *Phys. Chem. Chem. Phys.*, **12**, 2450-2458 (2010).
147. Q. Sun, S. Wang, H. Zhang, Z. Li, C. Pfisterer, S. Fischer, S. Nanbu and S.C. Smith, "Structural and Relaxation Effects in Proton Wire Energetics: Model Studies of the Green Fluorescent Protein Photocycle," *Aust. J. Chem.*, **63**, 363-370 (2010).
146. G. Liu, C. Sun, H.G. Yang, S.C. Smith, G.Q. Lu and H.M. Cheng "Nanosized Anatase TiO₂ Single Crystals for Enhanced Photocatalytic Activity," *Chem. Comm.*, **46**, 755-757 (2010).
145. Craig A. Bell, Qiao Sun, Hong Zhang, Sean C. Smith, Paul V. Bernhardt, Michael J. Monteiro, "Methyl Acrylate Polymerizations in the Presence of a Copper/N₃S₃ Macrobicyclic Cage in DMSO at 25 °C," *Polymer Chemistry*, **1**, 207-212 (2010).
144. A.J. Du, Y. Chen, Z.H. Zhu, R. Amal, G.Q. Lu, S.C. Smith, "Dots versus Antidots: Computational Exploration of Structure, Magnetism and Half-metallicity in Boron-Nitride Nanostructures," *J. Amer. Chem. Soc.*, **131**, 17354-17359 (2009).
143. P.G. Jambrina, F.J. Aoiz, N. Bulut, S.C. Smith, G.G. Balint-Kurti and M. Hankel, "The dynamics of the H⁺+D₂ reaction: A Comparison of Quantum Mechanical Wavepacket, Quasi-classical and Statistical-quasi-classical Results," *Phys. Chem. Chem. Phys.*, **12**, 1102-1115 (2010).
142. H. Yang, K.-L. Han, G. C. Schatz, S. C. Smith, M. Hankel, "Quantum Mechanical Calculations of the S(1D)+HD Reaction Dynamics on the Ground Electronic State," *J. Phys.: Conf. Ser.*, **185**, 012056 (4 pages) (2009).
141. H. Yang, K.-L. Han, G. C. Schatz, S. H. Lee, K. Liu, S. C. Smith and M. Hankel, "Integral and Differential Cross Sections for the S(1D)+HD Reaction Employing the Ground Adiabatic Electronic State," *Phys. Chem. Chem. Phys.*, **11**, 11587-11595 (2009).
140. A.J. Du, C.H. Sun, G.Q. Lu, V. Rudolph, Z.H. Zhu, S.C. Smith, "The Effect of Fe Doping on Adsorption of CO₂/N₂ within Carbon Nanotubes: A Density Functional Theory Study with Dispersion Corrections," *Nanotechnology*, **20**, 375701 (2009).
139. H. Zhang, S. Wang, Q. Sun and S.C. Smith, "Kinetic Isotope Effect for Ground State Proton Transfer in the Green Fluorescent Protein: A Quantum-Kinetic Model," *Phys. Chem. Chem. Phys.*, **11**, 8422-8424 (2009) (selected as PCCP "hot article").
138. D. Ouyang, H. Zhang, D.P. Herten, H.S. Parekh and S.C. Smith, "Flexibility of Short-Strand RNA in Aqueous Solution as Revealed by Molecular Dynamics Simulation: Are A-RNA and A'-RNA Distinct Conformational Structures?" *Aust. J. Chem.*, **62**, 1054-1061 (2009).
137. G. Liu, C.H. Sun, L. Cheng, Y.G. Jin, H.F. Lua, L.Z. Wang, S.C. Smith, G.Q. Lu, H.M. Cheng, "Efficient Promotion of Anatase TiO₂ Photocatalysis via Bifunctional Surface-Terminating Ti-O-B-N Structures," *J. Phys. Chem. C.*, **113**, 12317-12324 (2009).
- *136. T.J. Frankcombe and S.C. Smith, "Numerical Solution Methods for Large, Difficult Kinetic Master Equations," *Theor. Chem. Act.*, **124**, 303-317, (2009).

135. D. Ouyang, N. Shah, H. Zhang, S.C. Smith and H. Parekh, "Reducible Disulphide-Based Non-Viral Gene Delivery Systems," *Mini Reviews in Medicinal Chemistry*, **9**, 1242-1250 (2009).
134. G. Liu, C.H. Sun, X.X. Yan, L. Cheng, Z.G. Chen, X.W. Wang, L.Z. Wang, S.C. Smith, G.Q. Lu and H.M. Cheng, "Iodine Doped Anatase TiO₂ Photocatalyst with Ultra-long Visible Light Response: Correlation between Geometric/Electronic Structures and Mechanisms," *J. Mater. Chem.*, **19**, 2822-2829 (2009).
133. G. Liu, L.Z. Wang, C.H. Sun, X.X. Yan, X.W. Wang, Z.G. Chen, S.C. Smith, H.M. Cheng, G.Q. Lu, "Band-to-Band Visible-Light Photon Excitation and Photoactivity Induced by Homogeneous Nitrogen Doping in Layered Titanates," *Chem. Mat.*, **21**, 1266-1274 (2009).
132. H.G. Yang, G. Liu, S.Z. Qiao, C.H. Sun, Y.G. Jin, S.C. Smith, J. Zou, H.M. Cheng, G.Q. Lu, "Solvothermal Synthesis and Photoreactivity of Anatase TiO₂ Nanosheets with Dominant {001} Facets," *J. Amer. Chem. Soc.*, **131**, 4078-4083 (2009).
131. A.J. Du, Y. Chen, Z.H. Zhu, G.Q. Lu and S.C. Smith, "C-BN Single Walled Nanotubes from Hybrid Connection of BN/C Nanoribbons: Prediction by Ab Initio Density Functional Calculations," *J. Amer. Chem. Soc., rapid communication*, **131**, 1682-1683 (2009).
130. A.J. Du, Y. Chen, Z.H. Zhu, G.Q. Lu and S.C. Smith, "First Principle Studies of Zigzag AlN Nanoribbon," *Chem. Phys. Lett.*, **469**, 183-185 (2009).
129. A.J. Du, Z.H. Zhu, C.H. Sun, Y. Chen, G.Q. Lu, S.C. Smith, "Half Metallicity in a Zigzag Double Walled Nanotube Nanodot: an *ab initio* Prediction," *Chem. Phys. Lett.*, **468**, 257-259 (2009).
128. H. Yang, K. Han, S. Nanbu, H. Nakamura, G.G. Balint-Kurti, H. Zhang, S.C. Smith and M. Hankel, "Boltzmann averaged branching ratios and vibrational distributions for the O(¹D)+HCl → OH+Cl (OCl+H) reaction," *J. Theor. Comp. Chem.*, **8**, 1003-1024 (2009).
127. H. Zhang, Z.P. Xu, G.Q. Lu and S.C. Smith, "Intercalation of Sulfonate into Layered Double Hydroxide: Comparison of Simulation with Experiment," *J. Phys. Chem. C*, **113**, 559-566 (2009).
126. H. Zhang, S.C. Smith, S. Nanbu and H. Nakamura, "Quantum Mechanical Study of Atomic Hydrogen Interaction with Fluorinated Boron-Substituted Coronene Radical," *J. Phys. Condens. Matt.*, **21**, 144209 (8 pages) (2009).
125. L. Li, X.D. Yao, C.H. Sun, A.J. Du, L. Cheng, Z.H. Zhu, C.Z. Yu, J. Zou, S.C. Smith, P. Wang, H.M. Cheng, R.L. Frost and G.Q. Lu, "Lithium-Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage," *Advanced Functional Materials*, **19**, 265-271 (2009).
- *124. A.J. Du, S.C. Smith, C.H. Sun, L. Li, X.D. Yao and G.Q. Lu, "First Principle Study of Hydrogenation of MgB₂: An Important Step toward Reversible Hydrogen Storage in the Coupled LiBH₄/MgH₂ System," *J. Nanosci. Nanotech.*, (MPA2008), **9**, 4388-4391(2009).
123. P. Bargueno, T. Gonzalez-Lazana, P. Larregaray, L. Bonnet, J.C. Rayez, M. Hankel, S.C. Smith and A.J.H.M. Meijer, "Study of the H+O₂ Reaction by means of Quantum Mechanical and Statistical Approaches: The Dynamics on Two Different Potential Energy Surfaces," *J. Chem. Phys.*, **128**, 244308 (14 pages) (2008).
122. A. Du, S.C. Smith, X.D. Yao, C.H. Sun, L.Li and G.Q. Lu, "The Role of V₂O₅ on the Dehydrogenation and Hydrogenation in Magnesium Hydride: an *ab initio* Study," *Applied Physics Letters*, **92**, 163106 (3 pages) (2008).
121. H. Yang, K.L. Han, S. Nanbu, H. Nakamura, G.G. Balint-Kurti, H. Zhang, S.C. Smith and M. Hankel, "Energy Dependence of Branching Ratios and Product State Distributions for the O(¹D)+HCl reaction," *J. Phys. Chem. A*, **112**, 7947-7960 (2008).
120. H. Zhang, M. Hankel, S. Nanbu, H. Nakamura and S.C. Smith, "Quantum Calculation of Ro-vibrational States: Methodology and DOCl Application Results," *J. Phys Chem A*, **112**, 4141-4147 (2008).

119. C.H. Sun, X.D. Yao, A.J. Du, L. Li, S.C. Smith, G.Q. Lu, "Computational Study of Methyl Derivatives of Ammonia Borane for Hydrogen Storage," *Phys. Chem. Chem. Phys.*, **10**, 6104-6106 (2008).
118. A.J. Du, Y. Chen, G.Q. Lu and S.C. Smith, "Half-Metallicity in Finite-length Single Walled Zigzag Carbon Nanotubes: A First Principle Prediction," *Applied Physics Letters*, **93**, 073101 (3 pages) (2008) [[article featured on front cover](#)].
117. H.G. Yang, C.H. Sun, S.Z. Qiao, J. Zhou, S.C. Smith, H.M. Cheng and G.Q. Lu, "Anatase TiO₂ Single Crystals with a Large Percentage of {001} Facets," *Nature*, **453**, 638-641 (2008).
116. S. Olsen and S.C. Smith, "Bond Selectivity in the Photoisomerisation Reactions of Model GFP and KFP Chromophore Anions," *J. Amer. Chem. Soc.*, **130**, 8677-8689 (2008).
115. S.P. Nighswander-Rempel, S. Olsen, I.B. Mahadevan, G. Natchev, B.C. Wilson, S.C. Smith, H. Rubinsztein-Dunlop and Paul Meredith, "Effect of Dimerisation on Vibrational Spectra of Melanin Pre-cursors," *Photochem. Photobiol.*, **84**, 613-619 (2008).
114. M. Hankel, S.C. Smith, S.K. Gray and G.G. Balint-Kurti, "DIFFREALWAVE: A Parallel Real Wavepacket Code for the Quantum Mechanical Calculation of Reactive State-to-state Differential Cross Sections in Atom Plus Diatom Collisions," *Comput. Phys. Commun.*, **179**, 569-578 (2008).
113. P. Tran, H. Zhang, S.C. Smith, Y. Wong, Z.P. Xu and G.Q. Lu, "Molecular Dynamic Simulations of Interactions between LDH and NO₃⁻ Intercalates in Aqueous Solution.," *J. Phys. Chem. Solid.*, **69**, 1044-1047 (2008).
112. H. Yang, K.-L. Han, S. Nanbu, H. Nakamura, G.G. Balint-Kurti, H. Zhang, S.C. Smith and M. Hankel, "Quantum Dynamics Study of the O(¹D)+HCl Reaction Employing Three Electronic States," *J. Chem. Phys.*, **128**, 014308 (5 pages) (2008).
- *111. A.J. Du, Sean C. Smith and G.Q. Lu, "Surface Interactions of a Ti Atom with Sodium Alanate: an *ab initio* Spin-polarized Study," (invited paper for the 2006 Australia - Brazil Bio Nanotechnology Conference) *Int. J. Nanotech.*, **4**, 564-573 (2007).
110. A. Du, S.C. Smith and G.Q. Lu, "Formation of Single Walled Carbon Nanotube via the Interaction of Graphene Nanoribbons: *ab initio* Density Functional Calculations," *Nano Lett.*, **7**, 3349-3354 (2007).
109. A. Du, S.C. Smith and G.Q. Lu, "First Principle Studies of Electronic Structure and C-doping effect in Boron Nitride Nanoribbon," *Chem. Phys. Lett.*, **447**, 181-186 (2007) [selected as "Editor's Choice" article featured on front cover].
108. H. Zhang and S.C. Smith, "Model Real-Time Quantum Dynamical Simulations of Proton Transfer in the Green Fluorescent Protein (GFP)," *J. Theor. Comput. Chem.*, **6**, 789-802 (2007).
107. X. Yao, C.Z. Wu, A.J. Du, J. Zou, Y. He, Z.H. Zhu, P. Wang, H.M. Cheng, S.C. Smith, G.Q. Lu, "Metallic and Carbon Nanotube-Catalyzed Coupling of Hydrogenation in Magnesium," *J. Amer. Chem. Soc.*, **129**, 15650-15654 (2007).
106. A. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "Hydrogen Spillover Mechanism on a Pd-doped Mg Surface as Revealed by *ab initio* Density Functional Calculations," *J. Amer. Chem. Soc.*, **129**, 10201-10204 (2007).
105. A. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "The Role of Lithium Vacancies in Accelerating the Dehydrogenation Kinetics on a LiBH₄(010) Surface: an *ab initio* Study," *J. Phys. Chem. C*, **111**, 12124-12128 (2007).
104. A. Du, S.C. Smith and G.Q. Lu, "The Catalytic Role of Ti in the Dissociation of H₂ on a Ti-doped Al(001) Surface: an *ab initio* Density Functional Calculation," *Chem. Phys. Lett.*, **450**, 80-85 (2007).

103. B.Wanno, A.J.Du, V. Ruangpornvisuti, S.C. Smith, "Addition of Diazomethane to Armchair Single-walled Carbon Nanotubes and Their Reaction Sequences: A Theoretical Prediction," *Chem. Phys. Lett.*, **436**, 218 – 223 (2007).
102. S. Olsen, J. Riesz, I. Mahadevan, A. Coutts, B.J. Powell, R.H. Mckenzie, S.C. Smith and P. Meredith, "Convergent Proton Transfer Photocycles Violate Mirror-Image Symmetry in a Key Melanin Monomer," *J. Amer. Chem. Soc. rapid communication*, **129**, 6672-6673 (2007).
101. M. Hankel, S.C. Smith and A.J.H.M. Meijer, "State-to-State Reaction Probabilities for the $H+O_2(v, j) \rightarrow O+OH(v', j')$ Reaction on Three Potential Energy Surfaces," *J. Chem. Phys.*, **127** 064316 (10 pages) (2007).
100. J. Battad, P.G. Wilmann, S. Olsen, E. Byres, S.C. Smith, K. Turcic, R.J. Devenish, J. Rossjohn and M. Prescott "The Structural Basis for Increased Fluorescence Efficiency of the Chromoprotein Rtns5 at High pH," *J. Molec. Biol.*, **368**, 998 – 1010 (2007).
99. A.J. Du, Sean C. Smith and G.Q. Lu, "Vacancy Assisted Desorption of Hydrogen from a Sodium Alanate Surface: an *ab initio* Study," *Appl. Phys. Lett.*, **90**, 143119 (3 pages) (2007).
98. S. Wang and Sean C. Smith, "Mechanistic Aspects of Proton Chain Transfer in the Green Fluorescent Protein. II: A Comparison of Minimal Quantum Chemical Models," *Phys. Chem. Chem. Phys.*, **9**, 452-458 (2007) (front cover feature, Issue 4, 2007).
97. A.J. Du, Sean C. Smith and G.Q. Lu, "First Principle Studies of the Formation and Diffusion of Hydrogen Vacancies in Magnesium Hydride," *J. Phys. Chem. C*, **111**, 8360-8365 (2007).
96. Seth Olsen and Sean C. Smith, "Radiationless Decay of Red Fluorescent Protein Chromophore Models via Twisted Intramolecular Charge-Transfer States," *J. Amer. Chem. Soc.*, **129**, 2054 – 2065 (2007).
- *95. T.J. Frankcombe and S.C. Smith, "OH-initiated oxidation of toluene. II. Master Equation Simulation of Toluene Oxide Isomerisation," *J. Phys. Chem. A*, **111**, 3691-3696 (2007). (invited contribution to the special edition in honour of J. Miller's 60th birthday).
- *94. T.J. Frankcombe and S.C. Smith, "OH-initiated Oxidation of Toluene. I. Quantum Chemistry Investigation of the Reaction path," *J. Phys. Chem. A*, **111**, 3686 – 3690 (2007). (invited contribution to the special edition in honour of J. Miller's 60th birthday).
- *93. H. Zhang, S.C. Smith, S. Nanbu and H. Nakamura, "HOCl Ro-vibrational Bound State Calculations for Non-Zero Total Angular Momentum," *J. Phys. Chem. A*, **110**, 5468-5474 (2006) (invited contribution to the special edition in honour of Prof. J.C. Light's 65th birthday).
- *92. H. Zhang and S.C. Smith, "HO₂ Ro-vibrational State Calculations for Large Angular Momentum: $J = 30, 40,$ and 50 ," *J. Phys. Chem. A*, **110**, 3246-3253 (2006) (invited contribution to special edition in honour of Professor Jürgen Troe's 65th birthday).
- *91. S. Wang and S.C. Smith, "Leading Coordinate Analysis of Reaction Pathways in Proton Chain Transfer: Application to a Two-proton Transfer Model for the Green Fluorescent Protein," *Chem. Phys.*, (invited contribution to special edition in honour of 80th birthday of Professor Noel Hush), **326**, 204-209 (2006).
- *90. P. Wilmann, J. Battad, T. Beddoe, S. Olsen, S. Smith, S. Dove, R. Devenish, J. Rossjohn and M. Prescott, "The 2.0Å Crystal Structure of a Pocilloporin at pH 3.5: the Structural Basis for the Linkage of Colour Transition to Binding of Halides," *Photochemistry and Photobiology*, **82**, 359-366 (2006).
89. Marlies Hankel, Sean C. Smith, Robert J. Allan, Stephen K. Gray and Gabriel G. Balint-Kurti, "State-to-state Reactive Differential Cross Sections for the $H + H_2 \rightarrow H_2 + H$ Reaction on Five Different Potential Energy surfaces Employing a New Quantum Wavepacket Computer Code; DiffRealWave.," *J. Chem. Phys.*, **125**, 164303 (2006) (12 pages).

88. A. Du and Sean C. Smith, "Structural and Electronic Properties of Diazonium Functionalized (4, 4) Single Walled Carbon Nanotube: an ab initio Study," *Molecular Simulation*, **32**, 1213–1217 (2006).
87. A. Du, Sean C. Smith, X.D. Yao and G.Q. Lu, "First Principle Study of Adsorption of Hydrogen Molecules on Ti-doped Mg(0001) Surface," *J. Phys. Chem. B*, **110**, 21747 – 21750 (2006).
86. A.J. Du, G.Q. Lu and Sean C. Smith, "Role of Charge in Destabilizing AlH_4 and BH_4 Complex Anions for Hydrogen Storage Applications: Ab initio Density Functional Calculations," *Phys. Rev. B rapid communication*, **74**, 193405 (4 pages) (2006).
85. Seth Olsen and Sean C. Smith, "Trans-Cis Isomerism and Acylimine Formation in DsRed Chromophore Models: Intrinsic Rotation Barriers," *Chem. Phys. Lett.*, **426**, 159-162 (2006).
84. S.C. Olsen, M. Prescott, P. Wilmann, J. Battad, J. Rossjohn and Sean C. Smith "Determination of Chromophore Charge States in the Low pH Color Transition of the Fluorescent Protein Rtms5H146S via Time-Dependent DFT," *Chem. Phys. Lett.*, **420**, 507-511 (2006).
83. X. Yao, C.Z. Wu, A.J. Du, G.Q. Lu, H.M. Cheng, S.C. Smith, J. Zou and Y. He, "Mg-based Nanocomposites with High Capacity and Fast ad/Desorption Kinetics for Hydrogen Storage," *J. Phys. Chem. B.*, **110**, 11697 - 11703 (2006).
82. A.J. Du, Sean C. Smith, X.D. Yao, Y. He and G.Q. Lu, "Atomic Hydrogen Diffusion in Novel Magnesium Nanostructures: The Impact of Incorporated Subsurface Carbon Atoms," Asian Consortium for Computational Materials Science Symposium proceedings, *Journal of Physics: Conference Series*, **29**, 167-172 (2006).
81. L.M. Kettle, H.S. Goan and S.C. Smith, "Molecular orbital calculations of two-electron states for P donor solid-state spin qubits," *Phys. Rev. B*, **73**, 115205 (14 pages) (2006).
80. A.J. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "Ab initio Studies of Hydrogen Desorption from Low Index Magnesium Hydride Surface," *Surf. Sci.*, **600**, 1854-1859 (2006).
79. S. Wang and S.C. Smith, "Mechanistic Aspects of Proton Chain Transfer: A Computational Study for the Green Fluorescent Protein Chromophore," *J. Phys. Chem. B.*, **110**, 5084-5093 (2006).
78. A.J. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "Catalytic Effects of Sub-Surface Carbon in the Chemisorption of Hydrogen on a Mg(0001) Surface: an Ab-Initio Study," *J. Phys. Chem. B*, **110**, 1814-1819 (2006).
77. A.J. Du, S.C. Smith, X.D. Yao and G.Q. Lu, "The Role of Ti as a Catalyst for the Dissociation of H_2 on a Mg(0001) Surface," *J. Phys. Chem. B*, **109**, 18037-18041 (2005).
76. H. Zhang and S.C. Smith, "Unimolecular Ro-vibrational Bound and Resonance States for Large Angular Momentum: $J = 20$ Calculations for HO_2 ," *J. Chem. Phys.*, **123**, 014308 (9 pages) (2005).
75. A.J. Du and S.C. Smith, "Van der Waals-corrected Density Functional Theory: Benchmarking for Hydrogen-Nanotube and Nanotube-Nanotube Interactions," *Nanotechnology*, **16**, 2118-2123 (2005).
74. P.G. Wilmann, J. Petersen, A.Z. Pettikiriachchi, A.M. Buckle, S.C. Smith, S. Olsen, M.A. Perugini, R.J. Devenish, M. Prescott and J. Rossjohn, "The 2.1 Å Crystal Structure of the Far-red Fluorescent Protein HcRed: Inherent Conformational Flexibility of the Chromophore.," *J. Molecular Bio.*, **349**, 223-237 (2005).
- *73. H. Zhang and S.C. Smith, "Symmetry Contaminations in Reactive Scattering through Long-Lived Collision Complexes," *Chem. Phys.*, **308**, 297-304 (2005) (special memorial edition in honour of Gert du Billing).
72. A.C. Olleta, S.I. Lane and S.C. Smith, "Transition-State-Theory Calculations for Reactions of $\text{O}(^3P)$ with Halogenated Olefins," *Phys. Chem. Chem. Phys.*, **6**, 5362-5369 (2004).
71. T.J. Frankcombe and S.C. Smith, "On the Mechanism of Carbon Gasification: A Theoretical Study," *Carbon*, **42**,

2921-2928 (2004).

70. Z.H. Zhu, G.Q. Lu and S.C. Smith, "Comparative Study of Hydrogen Storage in Li- and K-doped Carbon materials - theoretically revisited," *Carbon*, **42**, 2509-2514 (2004).
69. V.V. Kislov, T.L. Nguyen, S.H. Lin, A.M. Mebel and S.C. Smith, "Photodissociation of Benzene under Collision-free Conditions: An Ab Initio/RRKM Study," *J. Chem. Phys.*, **120**, 7008-7017 (2004).
68. A.J. Rasmussen and Sean C. Smith, "A Lanczos-Powered Implementation of the Faber Polynomial Quantum Time Propagator for Reaction Probabilities," *Chem. Phys. Lett.*, **387**, 277-282 (2004).
67. H. Zhang and S.C. Smith, "Converged Quantum Calculations of HO₂ Bound States and Resonances for $J = 6$ and 10 ," *J. Chem. Phys.*, **120**, 9583-9593 (2004).
66. H. Zhang and S.C. Smith, "Iterative Quantum Computations of HO₂ Bound States and Resonances for $J = 4$ and 5 ," *Phys. Chem. Chem. Phys.*, **6**, 4240-4246 (2004).
65. H. Zhang and S.C. Smith, "Full S Matrix Calculation via a Single Real-Symmetric Lanczos Recursion: The Lanczos ABI Method," *J. Chem. Phys. (rapid communication)*, **120**, 1161-1163 (2004).
64. L.M. Kettle, H.-S. Goan, Sean C. Smith, L.C.L. Hollenberg and C.J. Wellard, "Effects of J -Gate Potential and Interfaces on donor exchange coupling in the Kane quantum computer architecture," *J. Phys: Condens. Matter* **16**, 1011-1023 (2004).
- *63. Hong Zhang and Sean C. Smith, "A Comparative Study of Iterative Chebyshev and Lanczos Implementations of the Boundary Inhomogeneity Method for Quantum Scattering," *J. Theor. Comput. Chem.* **2**, 563-572 (2003) (refereed manuscript in association with invited presentation at ACS symposium on iterative methods in quantum dynamics, New Orleans, March 2003).
62. T.J. Frankcombe and S.C. Smith, "Fast, Scalable Master Equation Solution Algorithms. IV. Lanczos Iteration with Diffusion Approximation Preconditioned Iterative Inversion," *J. Chem. Phys.* **119**, 12741-12748 (2003).
61. T.J. Frankcombe and S.C. Smith, "Fast, Scalable Master Equation Solution Algorithms. III: Direct Time Propagation Accelerated by a Diffusion Approximation Preconditioned Iterative Solver," *J. Chem. Phys.* **119**, 12729-12740 (2003).
60. H. Zhang and S.C. Smith, "Calculation of Bound and Resonance States of HO₂ for Non-Zero Total Angular Momentum," *J. Chem. Phys.*, **118**, 10042-10050 (2003).
59. L.M. Kettle, H.S. Goan, S.C. Smith, L.C.L. Hollenberg, C.I. Pakes and C. Wellard, "A Numerical Study of Hydrogenic Effective Mass Theory for an Impurity P Donor in Si in the Presence of an Electric Field and Interfaces," *Phys. Rev. B*, **68**, 075317 (2003) (6 pages).
58. T.J. Frankcombe and S.C. Smith, "Selecting Methods for Solving Multi-well Master Equations," *J. Theor. Comput. Chem.*, **2**, 179-191 (2003).
57. D. Reignier and S.C. Smith, "A Real Symmetric Lanczos Subspace Implementation of Quantum Scattering using Boundary Inhomogeneities," *Chem. Phys. Lett.*, **366**, 390-397 (2002).
56. H. Zhang and S.C. Smith, "Chebychev Real Wave Packet Propagation: H + O₂ ($J = 0$) State-to-State Reactive Scattering Calculations," *J. Chem. Phys.*, **117**, 5174-5182 (2002).
55. H.W. Schranz, S.C. Smith, A.M. Mebel, and S.H. Lin "Prediction of Absolute Rate Coefficients and Product Branching Ratios for the C(³P) + Allene Reaction System," *J. Chem. Phys.* **117**, 7055-7067 (2002).
54. H. Zhang and S.C. Smith, "Lanczos Subspace Time-Independent Wavepacket Calculations of S (¹D) + H₂ Reactive Scattering," *J. Phys. Chem. A*, **106**, 6137-6142 (2002).

53. H. Zhang and S.C. Smith, "Calculation of Resonances and Product State Distributions for the Unimolecular Dissociation of H₂S," *J. Phys. Chem. A*, **106**, 6129-6136 (2002).
52. H. Zhang and S.C. Smith, "Efficient Time-Independent Wavepacket Scattering Calculations within a Lanczos Subspace: H+O₂ (*J*=0) State-to-State Reaction Probabilities," *J. Chem. Phys.* **116**, 2354-2360 (2002).
51. T. J. Frankcombe, S. Bhatia and S.C. Smith, "Ab Initio Modelling of Basal Plane Oxidation of Graphenes and Implications for Modelling Char Combustion," *Carbon*, **40**, 2341-2349 (2002).
- *50. T.J. Frankcombe, S.C. Smith, "Time-Dependent Master Equation Simulation of Complex Elementary Reactions in Combustion: Application to the Reaction of ¹CH₂ with C₂H₂ from 300-2000K." *Faraday Discussion* **119**, 159-171 (2001).
49. H. Zhang and S.C. Smith, "Calculation of Product State Distributions from Resonance Decay via Lanczos Subspace Filter Diagonalization: Application to HO₂," *J. Chem. Phys.* **115**, 5751-5758 (2001).
48. T.J. Frankcombe and S.C. Smith, "Time Evolution in the Unimolecular Master Equation at Low Temperatures: Full Spectral Solution with Scalable Iterative Methods and High Precision," *Comput. Phys. Comm.* **141**, 39-54 (2001).
47. H. Zhang and S.C. Smith, "A Comparison of Low-Storage Strategies for Spectral Analysis in Dissipative Systems: Filter Diagonalization in the Lanczos Representation and Harmonic Inversion of the Chebychev-Order-Domain Autocorrelation Function," *Chem. Phys. Lett.*, **347**, 211-219 (2001).
46. H. Zhang and S.C. Smith, "Lanczos Subspace Filter Diagonalization: Homogeneous Recursive Filtering and a Low-storage Method for the Calculation of Matrix Elements," *Phys. Chem. Chem. Phys.*, **3**, 2282 - 2288 (2001).
45. A.J. Rasmussen, S.J. Jeffrey and S.C. Smith, "Subspace Wavepacket Evolution with Newton Polynomials," *Chem. Phys. Lett.*, **336**, 149-155 (2001).
- *44. T.J. Frankcombe, S.C. Smith, K.E. Gates and S.H. Robertson, "A Master Equation Model for Bimolecular Reaction via Multi-well Isomerising Intermediates," *Phys. Chem. Chem. Phys.*, **2** (Special Issue on Molecular Reaction Dynamics: Experiment and Theory, ed. J.N.L. Connor), 793-803 (2000).
43. S.C. Smith, "Kinematic Factors in Transition State Theory with a Generalized Reaction Coordinate," *J. Phys. Chem. A*, **104**, 10489-10499 (2000).
42. T.J. Frankcombe and S.C. Smith, "Solving the Unimolecular Master Equation with a Weighted Subspace Projection Method," *J. Comput. Chem.*, **21**, 592-606 (2000).
41. J.T. Lin, J.M. Yuan, S.C. Smith and S.H. Lin, "Dissociation Dynamics of HeRh²⁺ in Field-Ion Microscopy," *Phys. Rev. B*, **61**, 9419-9426 (2000).
- *40. S.C. Smith, H.-G. Yu, C. Leforestier and J.-C. Rayez, "Optimal Spectral Filtering in a Finite Subspace: a Lanczos-Based Implementation," *Phys. Chem. Chem. Phys.*, **1** (Special Issue on Chemical Reaction Theory, ed. J.N.L. Connor), 1311-1316 (1999).
39. A.J. Rasmussen and S.C. Smith, "Circulants, Symmetry and Time-Independent Wavepacket Scattering," *Chem. Phys. Lett.*, **312**, 229-236 (1999).
38. S.C. Smith, "Classical Flux Integrals in Transition State Theory: Generalized Reaction Coordinates," *J. Chem. Phys.*, **111**, 1830-1842 (1999).
37. A.J. Rasmussen, K.E. Gates and S.C. Smith, "A Pseudo-spectral Algorithm for the Computation of Transitional-mode Eigenfunctions in Loose Transition States. II. Optimized Primary and Grid Representations," *J. Chem.*

- Phys.*, **110**, 1354-1364 (1999).
36. V. Szalay and S.C. Smith, "Application of Contracted Distributed Approximating Functions to Solving Vibrational Eigenvalue Problems," *J. Chem. Phys.*, **110**, 72-79 (1999).
 35. N. Marchand, J.C. Rayez and S.C. Smith, "Theoretical Study of the Reaction $\text{CH}(\text{X}^2\Pi) + \text{NO}(\text{X}^2\Pi)$. III. Determination of the Branching Ratios," *J. Phys. Chem. A* **102**, 3358-3367 (1998).
 34. H.G. Yu and S.C. Smith, "Calculation of Quantum Resonance Energies and Lifetimes via Quasi-Minimum Residual Filter Diagonalization," *Chem. Phys. Lett.* **283**, 69-76 (1998).
 33. H.G. Yu and S.C. Smith, "The Elimination of Lanczos Ghosting by MINRES Filter Diagonalization," *J. Comp. Phys.* **143**, 484-494 (1998).
 - *32. H.G. Yu and S.C. Smith, "The Calculation of Vibrational Eigenstates by MINRES Filter Diagonalization," *Ber. Bunsenges. Phys. Chem.* **101**, 400-406 (1997).
 - *31. H.G. Yu and S.C. Smith, "Restarted Krylov-Space Spectral Filtering," *Faraday Transactions*, **93** (Special Issue on Theory of Chemical Reactions, ed. D.C. Clary), 861-869 (1997).
 30. S.J. Jeffrey and S.C. Smith, "Calculation of Absolute Spectral Densities via Stochastic Trace Estimators of $\text{tr}\{\alpha E-H\}$," *Chem. Phys. Lett.* **278**, 345-351 (1997).
 29. H.G. Yu and S.C. Smith, "The Simulation of Outgoing-Wave Boundary Conditions via a Symmetrically-Damped Hermitian Hamiltonian Operator," *J. Chem. Phys.* **107**, 9985-9993 (1997).
 28. S.C. Smith, M.J. McEwan and J.I. Brauman, "The Reversibility Relationship in Collision-Complex-Forming Bimolecular Reactions," *J. Phys. Chem. A*, **101**, 7311-7314 (1997).
 27. K.E. Gates, S.H. Robertson, K. Maschhoff, S.C. Smith, M. Beazley and M.J. Pilling, "Multiple-Well Isomerization Diffusion Equation Solutions with a Shift-and-Invert Lanczos Algorithm," *J. Phys. Chem. A* **101**, 5765-5769 (1997).
 26. S.J. Jeffrey, S.C. Smith and D.C. Clary, "Calculation of the Vibrational Spectral Density of NO_2 via Density Correlation Functions," *Chem. Phys. Lett.* **273**, 55-61 (1997).
 25. S.H. Robertson, M.J. Pilling, K.E. Gates and S.C. Smith, "Application of Inverse Iteration to 2-Dimensional Master Equations," *J. Comput. Chem.* **18**, 1004-1010 (1995).
 24. E. W.-G. Diau and S.C. Smith, "Theoretical Investigation of the Potential Energy Surface for the NH_2+NO Reaction via Density Functional Theory and Ab Initio Molecular Electronic Structure Theory," *J. Chem. Phys.* **106**, 9236-9251 (1997).
 - *23. S.C. Smith, "Towards Quantum Mechanical Characterization of the Dissociation Dynamics of Ketene," *Faraday Discussion* **102**, 17-29 (1996).
 22. E. W.-G. Diau and S.C. Smith, "Calculation of the Temperature Dependence of Rate Coefficients and Branching Ratios for the NH_2+NO Reaction via Microcanonical Variational Transition State Theory," *J. Phys. Chem.* **100**, 12349-12354 (1996).
 21. S.C. Smith and S.J. Jeffrey, "On the Calculation of Absolute Spectral Densities," *J. Chem. Phys.* **105**, 4055-4064 (1996).
 20. S. Jeffrey, K.E. Gates and S.C. Smith, "Full Iterative Solution of the Two-Dimensional Master Equation for Thermal Unimolecular Reactions," *J. Phys. Chem.* **100**, 7090-7096 (1996).

19. S.C. Smith, "A Pseudo-Spectral Algorithm for the Computation of Transitional Mode Eigenfunctions in Loose Transition States," *Chem. Phys. Lett.* **243**, 359-366 (1995).
18. Y. Guo, S.C. Smith, C.F. Melius and C.B. Moore, "Kinetics and Product Branching Ratios for the Reaction HCO + NO₂," *J. Phys. Chem.* **99**, 7473-7481 (1995).
17. V.G. Anicich, A.D. Sen, M.J. McEwan and S.C. Smith, "A Comparison of an Experimental Unimolecular Lifetime Distribution with RRKM Theory," *J. Chem. Phys.* **100**, 5696 (1994).
16. S.C. Smith, "Flux Factors in Variational Transition State Theory," *J. Phys. Chem.* **98**, 6496 (1994).
15. S.C. Smith, "Rapid Algorithms for Variational RRKM Theory," *J. Phys. Chem.* **97**, 7034 (1993).
14. S.C. Smith, P.F. Wilson, M.J. McEwan, P. Sudkeaw, R.G.A.R. Maclagan, W.T. Huntress, and V.G. Anicich, "Statistical Modeling of Capture, Association and Exit Channel Dynamics in the CH₃⁺/CH₃CN System," *J. Chem. Phys.* **98**, 1944 (1993).
13. S.C. Smith, "Angular-Momentum Resolution in Transitional-Mode State Counting for Loose Transition States," *J. Chem. Phys.* **97**, 2406 (1992).
12. S.C. Smith and J. Troe, "Statistical Modelling of Ion-Molecule Electrostatic Capture," *J. Chem. Phys.* **97**, 5451 (1992).
11. M.J.T. Jordan, S.C. Smith and R.G. Gilbert, "Variational Transition State Theory: A Simple Model for Dissociation and Recombination Reactions of Small Species," *J. Phys. Chem.* **95**, 8685 (1991).
10. S.C. Smith, "Microscopic Rate Coefficients in Reactions with Flexible Transition States: Analysis of the Transitional-Mode Sum of States," *J. Chem. Phys.* **95**, 3404 (1991).
9. M. Moet-Ner and S.C. Smith, "Entropy Barriers to Proton Transfer," *J. Amer. Chem. Soc.* **113**, 862 (1991).
8. S.C. Smith, M.J. McEwan, K. Giles, N.G. Adams and D. Smith, "Unimolecular Decomposition of a Polyatomic Ion in a Variable-Temperature Selected-Ion-Flow-Drift Tube: Experiment and Theoretical Interpretation," *Int. J. Mass. Spect. Ion. Proc.* **96**, 77 (1990).
7. S.C. Smith, M.J. McEwan and R.G. Gilbert, "Microscopic Reaction Rates in Ion-Molecule Reactions: Effects of Uncoupled Modes," *J. Phys. Chem.* **93**, 8142 (1989).
6. S.C. Smith, M.J. McEwan and R.G. Gilbert, "The Relationship between Recombination, Chemical Activation, and Unimolecular Dissociation Rate Coefficients," *J. Chem. Phys.* **90**, 4265 (1989).
5. S.C. Smith, M.J. McEwan and R.G. Gilbert, "The Pressure Dependence of Ion-Molecule Association Rate Coefficients," *J. Chem. Phys.* **90**, 1630 (1989).
4. S.C. Smith and R.G. Gilbert, "Program FALLOFF: Calculation of Falloff Curves for Unimolecular and Recombination Reactions through Solution of the Master Equation," *Quantum Chemistry Program Exchange* **8**, 168 (1988).
3. S.C. Smith and R.G. Gilbert, "Angular Momentum Conservation in Multichannel Unimolecular Reactions," *Int. J. Chem. Kinet.* **20**, 979 (1988).
2. S.C. Smith and R.G. Gilbert, "Angular Momentum Conservation in Unimolecular and Recombination Reactions," *Int. J. Chem. Kinet.* **20**, 307 (1988).
1. J.S. Knight, C.G. Freeman, M.J. McEwan, S.C. Smith, N.G. Adams and D. Smith, "Production and Loss of HC₃N in Interstellar Gas Clouds: Some Relevant Laboratory Measurements," *Mon. Not. R. Ast. Soc.* **219**, 89 (1986).