Sean C. Smith

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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)

2011/8 –	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	Editorial Advisory Board, Journal of Physical Chemistry
2003–present	Editorial Board, Computer Physics Communications
2003–2011	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

2012	FAAAS – Elected Fellow, Americal Association for the Advancement of Science.
2007	Bessel Research Award of the Alexander von Humboldt Foundation, Germany
1999	FRACI - Elected Fellow, 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 Memoral Medal, Royal Australian Chemical Institue
1989 – 1991	Alexander Von Humboldt Research Fellowship, Alexander von Humboldt Foundation, Federal Republic of Germany

Publications (Over 200 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 CO_2 gas separation.*
   Quantum chemical calculations and ab initio molecular dynamics are used to explore the interactions of small gaseous species such as CO_2, N_2, H_2O, CH_4 and H_2 with different nanotube architectures in order to assess the degree of selectivity for CO_2 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., HO_2 and HOCl.

Mentorship:

Past Graduate Students (Ph.D. unless otherwise noted)

S. Jeffrey (1994-1998); A. Rasmussen (1996-1999); T. Frankcombe (1998-2001); L. Kettle (2001-2004); S. Windsor (2003-2009); R. Gollan (2003-2006); D. Ouyang (2008-2010); B. Wanno; K. Wong (2006-2009); H. Yang (2005-2009); Y. Jiao (2009-2012); P. Yao (MSc, 2009-2012); Y.Y. Ma (2009-2012).

Current Graduate Students

B. Wu

Past Research Associates

W.G.. Diao (1995-1996); H.G. Yu (1996-1997); D. Bruget (1996-1997); V. Szalay (1998-1999); A. Rasmussen (2000-2001); H. Schranz (2000-2001); D. Hagebaum-Reignier (2001-2002); T. Frankcombe (2002-2004); S. Wang (2002-2006); A. Olletta (2003-2004); S. Olsen (2004-2007); P. Tran (2004-2008); H. Zhang (1999-2010); A. Du (2004-2012); , T. Liao (2010-2012), M. Hankel (2004-2012), C. Sun (2008-2012), Q. Sun (2008-2012); H. Sun (2010-2011).

Current Research Associates

Changwon Park; Jia Zhou.

PUBLICATIONS

Sean Smith
Director, Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
Oak Ridge, Tennessee

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.

Papers are arranged in broad thematic areas.
Invited papers marked with an asterisk.
Journals with impact factor above 6 are highlighted in blue.

COMPUTATIONAL NANOTECHNOLOGY

199. B. Wu, W.R. Chen, T. Egami, X. Li, Y. Liu, Y.M. Wang, C. Do, L. Porcar, K.L. Hong, L. Liu, G.S. Smith, S.C. Smith, "Molecular dynamics and neutron scattering study of the dependence of polyelectrolyte dendrimer conformation on counterion behavior", *J. Chem. Phys.*, **137**, 064902 (2012).

198. Wu, B., Kerkeni, B., Egami, T., Do, C., Liu, Y., Wang, YM, Porcar, L, Hong, K.L., Smith, S.C. , Liu, E.L., Smith, G.S., Chen, W.R., "Structured water in polyelectrolyte dendrimers: Understanding small angle neutron scattering results through atomistic simulation", *J. Chem. Phys.*, **136**, 144901 (2012).

196. Z. Li , A. Du , Q. Sun , M. Aljada , L.N. Cheng , M.J. Riley , Z.H. Zhu , Z.X. Cheng , X.L. Wang , J. Hall , E. Krausz , S.Z. Qiao , S.C. Smith and G.Q. Lu "Cobalt-doped cadmium selenide colloidal nanowires", *Chem. Commun.*, **47**, 11894-11896 (2011).

195. T. Liao, C.H. Sun, D. Hulicova-Jurcakova and S.C. Smith, "How to Achieve Maximum Charge Carrier Loading on Heteroatom-Substituted Graphene Nanoribbon Edges: Density Functional Theory Study", *J. Mat. Chem.*, **22**, 13751-13755 (2012).

193. A. Du, S. Sanvito and S.C. Smith, "First-principles prediction of metal-free magnetism and intrinsic half-metallicity in graphitic carbon nitride", *Phys. Rev. Lett.* **108**, 197207 (2012).

192. T. Liao, C.H. Sun, A. Du, D. Hulicova-Jurcakova and S.C. Smith, "Charge Carrier Exchange at Chemically Modified Graphene Edges: a Density Functional Theory Study", *J. Mater. Chem.* (accepted Feb2012).

191. A. Du, S. Sanvito, Z. Li, D.W. Wang, Y. Jiao, T. Liao, Q. Sun, Y.H. Ng, Z.H. Zhu, R. Amal, S.C. Smith, "Hybrid Graphene and Graphitic Carbon Nitride Nanocomposite: Gap Opening, Electron-hole Puddle, Interfacial Charge Transfer and Enhanced Visible Light Response", *J. Amer. Chem. Soc.*, **134**, 4393-4397 (2012).

190. C. Sun, A. Du, X. Yao, and S. C. Smith, "Adsorption and Dissociation of Ammonia Borane Outside and Inside Single-Walled Carbon Nanotubes: A Density Functional Theory Study," *J. Phys. Chem. C* **115**(25) 12580 – 12585 (2011).

189. M. Hankel, Y. Jiao, A.J. Du, S.K. Gray and S.C. Smith, "Asymmetrically Decorated, Doped Porous Graphene as an Effective Membrane for Hydrogen Isotope Separation," *J. Phys. Chem. C* **116**, 6672-6676 (2012).

188. Z. Li, P.W. Yi, Q. Sun, H. Lei, H.L. Zhao, Z.H. Zhu, S.C. Smith, M.B. Lan and G.Q. Lu, "Ultrasmall Water-soluble and Biocompatible Magnetic Iron Oxide Nanoparticles as Positive and Negative Dual Contrast Agents," *Adv. Funct. Mat.* **22**, 2387-2393 (2012).

187. Y. Zheng, Y. Jiao, J. Chen, J. Liu, J. Liang, A.J. Du, W. Zhang, Z.H. Zhu, S.C. Smith, M. Jaroniek, G.Q. Lu and S.Z. Qiao, "Nanoporous Graphitic-C_3N_4@Carbon Metal-Free Electrocatalysts for Highly Efficient Oxygen Reduction," *J. Amer. Chem. Soc.* **133**(50) 20116-20119 (2011).

186. C.H. Sun and S.C. Smith, "Strong Interaction between Gold and Anatase TiO_2(001) Predicted by First Principle Studies," *J. Phys. Chem. C* **116**(5), 3524 – 3531 (2012).

185. C.H. Sun, T. Liao, G.Q. Lu and S.C. Smith, "The Role of Atomic Vacancy on Water Dissociation over Titanium Dioxide Nanosheet: A DFT Study," *J. Phys. Chem. C* **116** (3) 2477-2482 (2012).

182. C.H. Sun, Y. Jia, X.H. Yang, H.G. Yang, X. Yao, G.Q. Lu, A. Selloni and S.C. Smith, "Hydrogen Incorporation and Storage in Well-defined Nano-crystals of Anatase Titanium Dioxide," *J. Phys. Chem. C* **115**(51), 25590 – 25594 (2011).

181. V. Murthy, H.D. Smith, H. Zhang and S.C. Smith, "Molecular Modeling of Hydrotalcite Structure Intercalated with Transition Metal Oxide Anions," *J. Phys. Chem. C* **115**(46), 13673-13683 (2011).

180. Y. Jiao, A.J. Du, M. Hankel, Z.H. Zhu, V. Rudolph and S.C. Smith, "Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification," *Chem. Comm.* **47**, 11843-11845 (2011).

179. C.H. Sun, A. Selloni, A. Du and S.C. Smith, "Interaction of Water with Fluorine-covered Anatase TiO_2 (001) Surface," *J. Phys. Chem. C* **115**(34), 17092 – 17096 (2011).

177. A. Mukherjia, C.H. Sun, S.C. Smith, G.Q. Lu and L.Z. Wang, "Photocatalytic Hydrogen Production from Water Using N-doped $Ba_5Ta_4O_{15}$ Under Solar Irradiation," *J. Phys. Chem. C* **15**(31), 15674-15678 (2011).

175. 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* **175**, 271-275 (2011).

174. 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.*,**13**, 11325-11328 (2011).

173. 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.*, **2(8)**, 894 – 899 (2011).

172. 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*, **115** (13), 6004 – 6009 (2011).

171. 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).

170. 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. Commun.*, **47**, 6293-6295 (2011).

169. 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).

168. 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 $CsTaWO_6$ photocatalysts for hydrogen production from water under visible light," *J. Mat. Chem.*, **21**, 8871-8879 (2011).

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 CO_2 and N_2 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 C_3N_4," *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. Commun.*, **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 TiO_2 Single Crystals for Enhanced Photocatalytic Activity," *Chem. Commun.*, **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 CO_2/N_2 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(28)**, 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 TiO_2 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(7),** 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 TiO_2 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," *Adv. Funct. Mat.*, **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 MgB_2: An Important Step Toward Reversible Hydrogen Storage in the Coupled $LiBH_4/MgH_2$ 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 V_2O_5 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 TiO_2 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 NO_3^- 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(4-6)**, 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(33)**, 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 $LiBH_4$(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 H_2 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 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).

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