

Project leadership

In addition to the research and pedagogic projects listed above, I coordinated (2004-2005) a project sponsored by the European Commission's Asia-link program entitled 'Linking Asian and European Universities in Implementation of Sustainable Technology'.

I co-organised a conference on 'Multiscale modelling of polymer systems', Borås, 6-9 June 2005, was a primary organiser of the 'Sixth International Conference on the Science and Application of Nanotubes', Gothenburg, July, 2005, was a local committee member for ISSPIC13 (Gothenburg, June, 2006) and was a co-organiser of the carbon nanotube growth focus session at the APS meeting, Washington DC, April 2010.

Scientific expertise

My experience in chemistry and physics departments, both in Sweden and internationally, has introduced me to a broad spectrum of theoretical methods and provided me with a wide range of computational tools. I am thus able to select and develop the best method(s) to attack a specific scientific problem. For example, I have combined molecular dynamics, statistical models, electronic structure theory, direct dynamics and QM/MM methods to study chemical reactions with water and carbon clusters. I believe that the direct dynamics and QM/MM methods will become even more widely used, especially in the nanosciences. I also believe that bridging the micro- to macroscale modelling gap will become increasingly important as industries move towards high-technological, knowledge-based product development.

Internationalisation:

I have been involved in educational and research collaborations with, among others, USA, England, Indonesia, Japan, Ireland and South Africa. As from 2009 I coordinate internationalisation activities at the University of Borås.

Publications, patents and conferences:

Over ninety scientific and educational contributions, a patent application publication, several invited talks at international conferences and numerous invited seminars. H-index = 23 and over 1350 citations.

Teaching and supervision:

I have completed a course in 'Higher Education' (10 week equivalent), Aug 2002-Nov 2003. I coordinated the project 'Computer animations for active learning of chemical concepts' funded by the Council for the Renewal of Higher Education (2005-06).

I believe that internet-based teaching will become even more important in the future, and have developed a distance course in Sustainable Development.

I am involved in the development, teaching and examination of various chemistry and chemical engineering courses at university level (teaching experience in both South Africa and Sweden). These include Applied Surface Chemistry (3rd year and MSc engineering students) and Physical Chemistry (2nd year chemical engineering students).

I have taught general science to underprivileged students in South Africa.

I have supervised post-doctor, PhD, MSc, BSc (Hons) and diploma projects.

Outreach:

Several talks to the general public, e.g., 'Smart textiles' in 2005, 'Computer modelling as a research and education tool', 2007, 'Sustainable Development and Nanotechnology' 2007 (for high school students and industry) and 'Kolnanoteknologi' 2008/09/10 for rotary groups. 2) Three articles on the use of computer simulations for non-university audiences. 3) Appeared in local newspaper, magazines and on Swedish TV regarding nanotechnology (2005, 07, 11).

Publications

(over 1500 citations and H-index = 24)

Reviews, chapters in books/encyclopedias

1. 'Direct Dynamics Simulations of Reactive Systems' Kim Bolton, William L. Hase and Gilles H. Peslherbe, in *Modern Methods for Multidimensional Computations in Chemistry*; D.L. Thompson, Ed.; World Scientific: New Jersey, 1998, p. 143.
2. 'Integrating the Classical Equations of Motion' Kim Bolton and William L. Hase, in *Encyclopedia of Computational Chemistry*, P. von Rague Schleyer, Ed.; John Wiley and Sons: Chichester, 1998, p. 1357.
3. 'Computer Animations in Physical Chemistry' Kim Bolton, in *Shifting Perspectives in Engineering Education*, M. F. Christie, Ed.; C-SELT, Gothenburg, 2006, p. 171.

Patent

4. 'Handling of derivatised carbon nanotubes', Kim Bolton, Arne Rosén and Simon Gustavsson, submitted to Swedish patent office 2002-11-15, submitted to PRV 2003-11-13, application published 2005 (application terminated due to lack of funding).

Refereed and peer-reviewed articles in conference proceedings

5. 'HCl ionisation in ice clusters – a direct dynamics study', Kim Bolton, Marcus Svanberg and Jan B. C. Pettersson, in *The Physics and Chemistry of Clusters: Proceedings of Nobel Symposium 117*; E.E.B. Campbell and M. Larsson, Eds.; World Scientific: New Jersey, 2000, p. 325.
6. 'A comparison of PM3 semiempirical and B3LYP density functional methods for calculating carbon nanotube – hydrocarbon bond strengths', Kim Bolton, Simon Gustavsson and Arne Rosén, *Third IEEE Conference on Nanotechnology*, (2003) 615.
7. 'Direct dynamics and QM/MM methods for studying large chemical systems: environmental and technological applications', Kim Bolton, *AMMS Proceedings*, (2004) 54.
8. 'Changes in carbon nanotube electronic properties by collisions with inert gases', Kim Bolton, Arne Rosén, Hugo Romero and Peter C. Eklund, *AIP Conference Proceedings*, **723** (2004) 87.
9. 'MD Simulations of Catalytic Carbon Nanotube Growth: Important Features of the Metal-Carbon Interactions' Feng Ding, Arne Rosén and Kim Bolton, *AIP Conference Proceedings*, **723** (2004) 364.
10. 'Simulation of conjugated alkene phase equilibria using transferable united atom force fields', Tyrone McKnight, Deresh Ramjugernath, Peter Ahlström and Kim Bolton, *3rd International Conference; Computational Modeling and Simulation of Materials A*, (2005) 337.
11. 'Molecular dynamics study of iron cluster coalescence at sub-melting point temperatures', Feng Ding, Kim Bolton and Arne Rosén, *Clusters and Nano-assemblies, Physical and Biological Systems*, edited by P Jena, S N Khanna & B K Rao (Virginia Commonwealth University, Richmond, November 2003) *Proceeding of*

International Symposium on Clusters And Nano-Assemblies (ISCANA): Physical and Biological Systems, (2005) p59.

12. 'Thermodynamics of carbon in iron nanoparticles at low temperature: reduced solubility and size-induced nucleation of cementite' Stefano Curtarolo, Neha Awasthi, Wahyu Setyawan, Na Li, Aiqin Jiang, Elena Mora, Kim Bolton, Avetik R. Harutyunyan, *Physics Procedia* **6** (2010) 16.
13. 'Computational Studies of Binding Energies and Structures of Methylamine on Functionalized Activated Carbon Surfaces.' R. C. J. Mphahlele, K. Bolton and H. Kasaini, *World Academy of Science, Engineering and Technology* **71** (2010) 963.

Refereed Articles in Journals

General

14. 'The Potential Carcinogenic Effect of Uvinul DS49 --- a Common UV Absorber used in Cosmetics.' Kim Bolton, Bice S. Martincigh and Leo F. Salter, *J. Photochem. Photobiol. A: Chem*, **63** (1992) 241.
15. 'An Evaluation of the Gauss-Radau Algorithm for the Simulation of Chemical Dynamics.' Kim Bolton and Sture Nordholm, *J. Comput. Phys.*, **113** (1994) 320.

Intramolecular energy redistribution, unimolecular and bimolecular reactions

16. 'Vibrational Energy Transfer in a One-dimensional Chain of Diatomic Molecules', Kim Bolton and Sture Nordholm, *Chem. Phys.*, **182** (1994) 263
17. 'Fragmentation of One-Dimensional Monatomic Chains under Tension: Simulation and Statistical Theory', Kim Bolton, Sture Nordholm and Harold W. Schranz, *J. Phys. Chem.*, **99** (1995) 2477.
18. 'A Molecular Dynamics Study of the Intramolecular Energy Transfer and Isomerisation of Stilbene.' Kim Bolton and Sture Nordholm, *Chem. Phys.*, **203** (1996) 101.
19. 'Classical Dynamics Simulations of Model *Trans*-stilbene: Collisional Effects on Intramolecular Energy Transfer.' Kim Bolton and Sture Nordholm, *Chem. Phys.*, **206** (1996) 103.
20. 'The correspondence between the frequency of classical quasiperiodic energy flow and quantum beating.' Kim Bolton and Sture Nordholm, *Chem. Phys.*, **207** (1996) 63.
21. 'Direct Dynamics Study of the Lifetime of Trimethylene.' Charles Doubleday, Jr., Kim Bolton, Gilles H. Peslherbe and William L. Hase, *J. Am. Chem. Soc.*, **118** (1996) 9922.
22. 'Isomerisation of Deuterated Cyclopropanes: The Possibility for Stereochemical Control', Kim Bolton, William L. Hase and Charles Doubleday, Jr., *Ber. Bunsenges. Phys. Chem.*, **3** (1997) 414.
23. 'Direct Dynamics Study of the Stereomutation of Cyclopropane' Charles Doubleday, Jr., Kim Bolton and William L. Hase, *J. Am. Chem. Soc.*, **119** (1997) 5251.

24. 'Direct Dynamics Quasiclassical Trajectory Study of the Thermal Isomerisations of Cyclopropane' Charles Doubleday, Jr., Kim Bolton and William L. Hase, *J. Phys. Chem. A.*, **102** (1998) 3648.
25. 'A QM/MM Direct Dynamics Trajectory Investigation of Trimethylene Decomposition in an Argon Bath.' Kim Bolton, William L. Hase and Charles Doubleday, Jr., *J. Phys. Chem. B*, **103** (1999) 3691.
26. 'A Direct Dynamics Study of the $F + C_2H_4 \rightarrow C_2H_3F + H$ Product Energy Distributions' Kim Bolton, William L. Hase, H. Bernhard Schlegel and Kihyung Song, *Chem. Phys. Letters*, **288** (1998) 621.
27. 'An *Ab Initio* Quasiclassical Direct Dynamics Investigation of the $F + C_2H_4 \rightarrow C_2H_3F + H$ Product Energy Distributions.' Kim Bolton, William L. Hase, H. Bernhard Schlegel and Kihyung Song, *Phys. Chem. Chem. Phys.*, **1** (1999) 999.

Ice surfaces and water clusters

28. 'Classical trajectory study of argon-ice collision dynamics.' Kim Bolton, Marcus Svanberg and Jan B. C. Pettersson, *J. Chem. Phys.*, **110** (1999) 5380.
29. 'Trapping-Desorption and Surface Penetration of Ar on Ice.' Kim Bolton and Jan B. C. Pettersson, *Chem. Phys. Letters*, **312** (1999) 71.
30. 'Dynamics of Argon collisions with water ice: Molecular beam experiments and molecular dynamics simulations', Patrik U. Andersson, Matts B. Någård, Kim Bolton, Marcus Svanberg and Jan B. C. Pettersson, *J. Phys. Chem. A*, **104** (2000) 2681.
31. 'A molecular dynamics study of the long time ice Ih surface dynamics.' Kim Bolton and Jan B. C. Pettersson, *J. Phys. Chem. B*, **104** (2000) 1590.
32. 'Coupled QM/MM molecular dynamics simulations of HCl interacting with ice surfaces and water clusters – evidence of rapid ionization', Marcus Svanberg, Jan B. C. Pettersson and Kim Bolton, *J. Phys. Chem. A.*, **104** (2000) 5787.
33. 'Ice-catalysed ionisation of hydrochloric acid', Kim Bolton and Jan B. C. Pettersson, *J. Am Chem. Soc.*, **123** (2001) 7360.
34. 'A QM/MM study of HCl adsorption at ice defect sites', Kim Bolton, *J. Molec. Struct. Theochem*, **632** (2003) 145.
35. 'A semiempirical QM/MM method for studying HCl adsorption on ice', Kim Bolton, *Int. J. Quant. Chem.*, **96** (2004) 607.
36. 'Simulation of water vapour clusters in direct equilibrium with liquid water', Erik Johansson, Kim Bolton and Peter Ahlström, *Comput. Phys. Commun.*, **169** (2005) 54.
37. 'Simulations of vapor water clusters at vapor-liquid equilibrium', Erik Johansson, Kim Bolton and Peter Ahlström, *J. Chem. Phys.*, **123** (2005) 024504.
38. 'Argon collisions with amorphous water ice surfaces', Jan B. C. Pettersson, Martina T. Suter, Patrik U. Andersson and Kim Bolton, *Chem. Phys.*, **326** (2006) 281.

Metal and metal-carbide nanoclusters

39. 'Assessing the validity of theoretical results', Sven Varga, Kim Bolton, Henrik Grönbeck, Anders Snis, Arne Rosén and Burkhard Fricke, *European Physical Journal D*, **16** (2001) 29.
40. 'Iron-carbide cluster thermal dynamics for catalysed carbon nanotube growth', Feng Ding, Kim Bolton and Arne Rosén, *J. Am. Vac. Sci. Technol. A*, **22** (2004) 1471.

41. 'Size Dependence of the Coalescence and Melting of Iron Clusters: A Molecular Dynamics Study' Feng Ding, Arne Rosén and Kim Bolton, *Phys Rev. B.*, **70** (2004) 075416.
42. 'Molecular Dynamics Study of the Surface Melting of Iron Clusters', Feng Ding, Kim Bolton and Arne Rosén, *Eur. Physics J. D.*, **34** (2005) 275.
43. 'Structure and thermal properties of supported catalyst clusters for single-walled carbon nanotube growth', Feng Ding, Kim Bolton and Arne Rosén, *Appl. Surf. Sci.*, **252** (2006) 5254.
44. 'Modeling the Melting of Supported Clusters', F. Ding, A. Rosén, S. Curtarolo and K Bolton, *Appl. Phys. Letters*, **88** (2006) 133110.
45. 'Hidden features of the catalyst nanoparticles favorable for single-walled carbon nanotube growth', A. Harutyunyan, E. Mora, T. Tokune, A. Epstein, K. Bolton, A. Jiang, N. Awasthi and S. Curtarolo, *Appl. Phys. Letters*, **90** (2007) 163120.
46. 'Size dependent melting mechanisms of iron nanoclusters', Haiming Duan, Feng Ding, Arne Rosén, Avetik R. Harutyunyan, Stefano Curtarolo, Kim Bolton, *Chem. Phys.* **333** (2007) 57.
47. 'Theoretical study of the thermal behaviour of free and alumina-supported Fe-C nanoparticles', A. Jiang, N. Awasthi, A. N. Kolmogorov, W. Setyawan, A. Börjesson, K. Bolton, A. Harutyunyan and S. Curtarolo, *Phys. Rev. B* **75** (2007) 205426.
48. 'Computational studies of small carbon and iron-carbon systems relevant to carbon nanotube growth', Haiming Duan, Arne Rosén, Avetik Harutyunyan, Stefano Curtarolo and Kim Bolton, *J. Nanosci. Nanotech.*, **8** (2008) 6170.
49. 'Reduced carbon solubility in Fe nanocatalysts and implications for the growth of single walled carbon nanotubes', A. R. Harutyunyan, N. Awasthi, A. Jiang, W. Setyawan, E. Mora, T. Tokune, K. Bolton and S. Curtarolo, *Phys. Rev. Letters*, **100** (2008) 195502.
50. 'Computational study of the thermal behavior of iron clusters on a porous substrate', A. Börjesson, A. R. Harutyunyan, S. Curtarolo and K. Bolton, *Phys. Rev. B.*, **77** (2008) 115450.
51. 'Influence of Mo on the Fe:Mo:C nanocatalyst thermodynamics for single-walled carbon nanotube growth', S. Curtarolo, N. Awasthi, W. Setyawan, A. Jiang, K. Bolton, T. Tokune and A. R. Harutyunyan, *Phys. Rev. B* **78** (2008) 054105.
52. 'Computational studies of catalytic particles for carbon nanotube growth', Kim Bolton, Feng Ding, Anders Börjesson, Wuming Zhu, Haiming Duan, Arne Rosén, Avetik R. Harutyunyan and Stefano Curtarolo, *J. Comput. Theo. Nanosci.*, **6** (2009) 1.

Carbon nanoclusters

53. 'Computational studies of gas - carbon nanotube collision dynamics', Kim Bolton and Arne Rosén, *Phys. Chem. Chem. Phys.*, **4** (2002) 4481.
54. 'A theoretical analysis of ether-group derivatisation at carbon nanotube ends', Simon Gustavsson, Arne Rosén and Kim Bolton, *Nano Letters*, **3** (2003) 265.
55. 'Energy transfer mechanisms in gas – carbon nanotube collisions', Kim Bolton and Simon Gustavsson, *Chem. Phys.*, **291** (2003) 161.
56. 'Hydrocarbon derivatisation at carbon nanotube ends: effect of link heteroatom and hydrocarbon structure on tube-hydrocarbon bond strength' Simon Gustavsson, Arne Rosén, Helena Grennberg and Kim Bolton, *Chem. Eur. J.*, **10** (2004) 2223.

57. 'Thermal physics in carbon nanotube growth kinetics', Oleg A. Louchev, Hisao Kanda, Arne Rosén and Kim Bolton, *J. Chem. Phys.*, **121** (2004) 446.
58. 'Nucleation and Growth of Single-Walled Carbon Nanotubes: A Molecular Dynamics Study', Feng Ding, Kim Bolton and Arne Rosén, *J. Phys. Chem. B.*, **108** (2004) 17369.
59. 'Molecular Dynamics Study of the Catalyst Particle Size Dependence on Carbon Nanotube Growth', Feng Ding, Arne Rosén and Kim Bolton, *J. Chem. Phys.*, **121** (2004) 2775.
60. 'The role of the catalytic particle temperature gradient for SWNT growth from small particles' Feng Ding, Kim Bolton and Arne Rosén, *Chem. Phys. Lett.*, **393** (2004) 309.
61. 'Atom Collision-Induced Resistivity of Carbon Nanotubes', Hugo E. Romero, Kim Bolton, Arne Rosén and Peter C. Eklund, *Science*, **307** (2005) 89.
62. 'Dependence of SWNT growth mechanism on temperature and catalyst particle size: bulk versus surface diffusion', Feng Ding, Arne Rosén and Kim Bolton, *Carbon*, **43** (2005) 2215.
63. 'Molecular dynamics study of SWNT growth on catalyst particles without temperature gradients', Feng Ding, Kim Bolton and Arne Rosén, *Comp. Mat. Sci.*, **35** (2006), 243.
64. 'Molecular Dynamics Study of Bamboo-like Carbon Nanotube Nucleation', Feng Ding, Kim Bolton and Arne Rosén, *J. Elec. Mat.*, **35** (2006) 207.
65. 'Atomistic simulations of catalyzed carbon nanotube growth' Kim Bolton, Feng Ding and Arne Rosén, *J. Nanosci. Nanotech.*, **6** (2006) 1211.
66. 'The importance of a supersaturated carbon concentration and its distribution in catalytic metal particles for single-walled carbon nanotube nucleation', Feng Ding and Kim Bolton, *Nanotechnology* **17** (2006) 543.
67. 'Graphitic encapsulation of catalyst particles during carbon nanotube production', Feng Ding, Arne Rosén, Eleanor E.B. Campbell, Lena Falk and Kim Bolton, *J. Phys. Chem. B*, **110** (2006) 7666.
68. 'Calculating carbon nanotube – catalyst adhesion strengths', Peter Larsson, J. Andreas Larsson, Rajeev Ahuja, Feng Ding, Boris Yakobson, Haiming Duan, Arne Rosén and Kim Bolton, *Phys. Rev. B* **75** (2007) 115419.
69. 'Initial growth of single-walled carbon nanotubes on supported iron clusters: a molecular dynamics study' Haiming Duan, Feng Ding, Arne Rosén, Avetik Harutyunyan, Toshio Tokune, Stefano Curtarolo and Kim Bolton, *Eur. J. Phys. D.* **43** (2007) 185.
70. 'Changes in single wall carbon nanotube chirality during growth and regrowth', Wuming Zhu, Arne Rosén and Kim Bolton, *J. Chem. Phys.*, **128** (2008) 124708.
71. 'The importance of strong carbon-metal adhesion for catalytic nucleation of single-walled carbon nanotubes', Feng Ding, Peter Larsson, J. Andreas Larsson, Rajeev Ahuja, Haiming Duan, Arne Rosén and Kim Bolton, *Nano Letters*, **8** (2008) 463. (Reported as a 'Research Highlight' in *Nature Nanotechnology* - <http://www.nature.com/nnano/reshigh/2008/0108/full/nnano.2008.21.html>).
72. 'Diameter and Chirality Changes of Single-Walled Carbon nanotubes During Growth: An ab-initio Study', Wuming Zhu, Haiming Duan and Kim Bolton, *J. Nanosci. Nanotechnol.* **2** (2009) 1222.
73. 'Computational studies of metal-carbon nanotube interfaces for regrowth and electronic transport', Anders Börjesson, Wuming Zhu, Hakim Amara, Christophe Bichara and Kim Bolton, *Nano Letters*, **9** (2009) 1117.
74. 'DFT and Tight Binding based Dynamical Studies of Carbon-Metal Systems of Relevance to CNT Growth' Kim Bolton, Anders Börjesson, Wuming Zhu, Hakim Amara, Christophe Bichara, *Nano Research*, **2** (2009) 774.

75. 'DFT and tight binding Monte Carlo calculations related to single-walled carbon nanotube nucleation and growth', Wuming Zhu, Anders Börjesson, and Kim Bolton, *Carbon*, **48** (2010) 470.
76. 'First Principles Studies of the Effect of Nickel Carbide Catalyst Composition on Carbon Nanotube Growth', Anders Börjesson and Kim Bolton, *J. Phys. Chem. C*, **114** (2010) 18045.
77. 'First principles studies of the effect of Ostwald ripening on carbon nanotube distributions', Anders Börjesson and Kim Bolton, *ACS Nano* **5** (2011) 771.
78. 'Modelling of Ostwald ripening of metal clusters attached to carbon nanotubes' Anders Börjesson and Kim Bolton, *J. Phys. Chem. C*, **115** (2011) 24454.
79. 'Progress in understanding controlled single-wall carbon nanotube growth from computer simulations' Kim Bolton, Wuming Zhu and Anders Börjesson, *J. Comp. Theo. Nanosci.*, accepted.
80. 'Continuum-molecular modelling of graphene', Kaveh Samadikhah, Ragnar Larsson, Faranak Bazooyar and Kim Bolton, *Comp. Mat. Sci.*, **53** (2012) 37.
81. 'Computational studies of graphene growth mechanisms', Shayesteh Haghghatpanah' Anders Börjesson, Hakim Amara, Christophe Bichara and Kim Bolton, submitted.

Hydrocarbon and polymer systems

82. 'Comparison of explicit and united atom models for alkane chains physisorbed on α -Al₂O₃ (0001).' Kim Bolton, Sylvie Bosio, William L. Hase, William Schneider and Kenneth Hass, *J. Phys. Chem. B*, **103** (1999) 3885.
83. 'Simulating 1-alkene and alkane binary vapor-liquid equilibrium using different united-atom transferable force fields' Tyrone McKnight, Thijs Vlugt, Deresh Ramjugernath, Matthew Starzak, Peter Ahlström and Kim Bolton, *Fluid Phase Equilibria*, **232** (2005) 136.
84. 'Monte Carlo Simulation of Carboxylic Acid Phase Equilibria', Scott Clifford, Kim Bolton and Deresh Ramjugernath, *J. Phys. Chem. B*, **110** (2006) 21938.
85. 'Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene', Erik Johansson, Kim Bolton, Doros N. Theodorou and Peter Ahlström, *J. Chem. Phys.* **126** (2007) 224902.
86. 'Water absorption in polyethylene under external electric fields', Erik Johansson, Kim Bolton and Peter Ahlström, *J. Chem. Phys.* **127** (2007) 24902.
87. 'Formation of rod-like structures of water between oppositely charged ions in decane and polyethylene', Erik Johansson, Kim Bolton, Doros N. Theodorou and Peter Ahlström, *J. Chem. Phys.* **127** (2007) 191101.
88. 'Molecular simulation of the effect of ionic impurities and external electric fields on rod-like water clusters in polyethylene', Erik Johansson, Peter Ahlström and Kim Bolton, *Polymer* **49** (2008) 5357.
89. 'Simulation of water clusters in vapour, alkanes and polyethylenes' Kim Bolton, Erik Johansson, Lennart Jönsson and Peter Ahlström, *Mol. Sim.* **35** (2009) 888.
90. 'Gibbs ensemble Monte Carlo simulations of binary vapour-liquid-liquid equilibrium: application to n-hexane/water and ethane/ethanol systems', S. Moodley, E. Johansson, K. Bolton and D. Ramjugernath, *Mol. Sim.* **36** (2010) 758.
91. 'Monte Carlo simulations of vapor-liquid-liquid equilibrium of some ternary petrochemical mixtures' Suren Moodley, Kim Bolton and Deresh Ramjugernath, *Fluid Phase Equilibria* **299** (2010) 24.

92. 'Analysis of the torsion angle distribution of poly(vinylidene fluoride) in the melt', Kavitha Chelakara Satyanarayana, Martin Bohlén, Anja Lund, Rodney Rychwalski and Kim Bolton, *Polymer* **53** (2012) 1109.
93. 'Validating Empirical Force Fields for Molecular-level Simulation of Cellulose Dissolution', Faranak Bazooyar, Frank A. Momany and Kim Bolton, *Comput. Theo. Chem.* **984** (2012) 119.
94. 'Phase-dependent energy cross-parameters in a monatomic binary fluid system', S. Moodley, E. Johansson, K. Bolton and D. Ramjugernath, *Mol. Sim.*, accepted.
95. 'First principles and molecular mechanics studies of carbon nanotube – polyvinylidene systems', Martin Bohlén, Kavitha Chelakara Satyanarayana and Kim Bolton, manuscript.
96. 'Computer simulations of α - to β -poly (vinylidene fluoride) phase change by stretching and poling', Kavitha Chelakara Satyanarayana and Kim Bolton, submitted.
97. 'Simulation of α - and β -PVDF melting mechanisms', Edvin Erdtman, Kavitha Chelakara Satyanarayana and Kim Bolton, manuscript.

Peer-reviewed articles in popular science and engineering journals

98. 'Phase equilibrium by computer experiments', Tyrone McKnight, Deresh Ramjugernath, Kim Bolton and Peter Ahlström, *Chem. Tech.*, April (2002) 28.
99. 'Studying the dynamics of chemical systems by computer simulations – Part 2', Tyrone McKnight, Deresh Ramjugernath, Kim Bolton and Peter Ahlström, *Chem. Tech.*, November (2002) 29.

Peer-reviewed: Education in science and engineering

100. 'Molecular-level computer simulations in chemical engineering', Kim Bolton, *CREE*, **6** (2002) 3
101. 'North-South collaboration in technological advancement: the Sweden-South Africa Engineering Education Collaboration Project.' Zola Mbanguta, Kim Bolton, Göran Gustafsson, *World Trans. Eng. Tech. Edu.*, **1** (2002) 185.
102. 'SimChemistry as an active learning tool in chemical education', Kim Bolton, Michael Christie, Åke Ingerman, Cedric Linder, Elisabeth Saalman, *Chem. Educ. Res. Pract.*, **9** (2008) 277.

Technical reports, non-peer-reviewed conference articles and popular scientific articles

103. 'Computational studies of scattering from ice and carbon clusters', Kim Bolton, Arne Rosén and Martina Suter, *NSC Progress Report*, (2001) 22.
104. 'A theoretical study of carbon nanotube functionalization', Simon Gustavsson, Kim Bolton and Arne Rosén, *NSC Progress Report*, (2002) 24.
105. 'Computational studies of conductivity through molecular junctions', Peter Klason, Magnus Willander, Arne Rosén, Maria Tengelin-Nilsson, Janusz Kanski and Kim Bolton, *NSC Progress Report*, (2003) 85.

106. 'Computational study of catalyzed carbon nanotube growth', Feng Ding Arne Rosén and Kim Bolton, *SNIC Progress Report*, (2003-2005) 32.
107. 'A large interest in small things: carbon nanotube growth mechanisms', Kim Bolton, *NSC News*, December 2006.
108. 'Determination of binding energies of platinum ions on functionalized activated carbons through density functional theory', H. Kasaini, J. Mphahlele and K. Bolton, *Minerals Engineering International conference proceedings - 2009*
109. 'Beräkningsteknik: Användning inom energi och material för hållbar utveckling', Kim Bolton, Anders Börjesson, Faranak Bazooyar och Peter Ahlström, *The School of Engineering's 20th Jubilee Report, University of Borås*, October 2009.
110. 'Computational studies of single-walled carbon nanotube growth', Kim Bolton and Anders Börjesson, *SNIC Progress Report*, (2008-2009) 40.

Conference Presentations (presenting author underlined)

1. 'The Mathematical Simulation of the Movement of Solvated Electrons Through Various Media.' K. Bolton and L.F. Salter, South African Chemical Institute Seminar Presentations, Durban, October 1985.
2. 'Mechanism of Product Determination of the Photosensitised Reaction of Free Thymine Base.' K. Bolton, B.S. Martincigh and L.F. Salter, Tenth Congress: South African Biochemical Society, Pietermaritzburg, 29 January 1991.
3. 'Photosensitisation of Thymine Base in vitro and in vivo.' K. Bolton, B.S. Martincigh and L.F. Salter, Congress: South African Chemical Institute Grahamstown, 25 June 1991.
4. 'Stilbene Isomerisation: Reaction Mechanisms and Dynamics.' K. Bolton and S. Nordholm, EUCHEM Conference: Ultrafast Processes in Chemistry and Biology, Ulvoen, Sweden, 13 July 1994.
5. 'Stilbene Isomerisation: A computational investigation of the trans-cis reaction.' K. Bolton and S. Nordholm, Molecular Dynamics in the Gas Phase and at Interfaces, Kaiserslautern, Germany, 10 July 1995.
6. 'Direct Dynamics Study of Trimethylene.' K. Bolton, W. L. Hase and C. Doubleday, 39th Midwest Conference of Computational Chemistry, Indianapolis, USA, 30 May 1996.
7. 'F + C₂H₄ ---> C₂H₃F + H Product Energy Distributions.' K. Bolton, W. L. Hase, H. B. Schlegel and K. Song, Dynamics of Molecular Collisions, Gull Lake, USA, 20 June 1996.
8. 'Ar-ice collision dynamics.' K. Bolton, M. Svanberg and J. B. C. Pettersson, MOLEC, Bristol, England, 7 September 1998.
9. 'Computer simulations of ice Ih surface dynamics.' K. Bolton, M. Svanberg and J. B. C. Pettersson, Dynamics at Interfaces, Hindås, Sweden, 1 June 1999.
10. 'Stratospheric ionisation of HCl – a QM/MM study.' K. Bolton, M. Svanberg and J. B. C. Pettersson, DYNAM 2000, Arcachon, France, 31 May 2000.
11. 'HCl ionisation in ice clusters.' K. Bolton, M. Svanberg and J. B. C. Pettersson, Nobel Symposium on Cluster Physics, Visby, Sweden, 28 June 2000.
12. 'Direct dynamics and QM/MM simulations of chemical reactions.' K. Bolton and J. B. C. Pettersson, 4th national meeting on femtosecond spectroscopy and dynamics, Göteborg, Sweden, 28 September, 2000.
13. 'Computational studies of gas- carbon nanotube collision dynamics', Kim Bolton and Arne Rosen, 41st Sanibel Symposium, Florida, USA, 24 February - 2 March 2001.
14. 'Computer simulations of diffusion on ice surfaces', K. Bolton, J. B. C. Pettersson and A. Rosén, Conference of the American Physical Society, Seattle, USA, 12 March 2001.
15. 'Computational studies of catalysed nanotube growth'. K. Bolton, D. Bozi and A. Rosén, NT01, Potsdam, Germany, 22 July 2001.
16. 'Gas - carbon nanotube collision dynamics', Kim Bolton and Arne Rosén, The 7th International Conference on Nanometer-Scale Science and Technology and the 21st European Conference on Surface Science, Malmö, Sweden, 24-28 June, 2002.
17. 'Gas – carbon nanotube collision dynamics.' K. Bolton, S. Gustavsson and A. Rosén, NT02, Boston, USA, 6 July 2002.
18. 'Thermal vibrations of and scattering off carbon nanotubes' Arne Rosen and Kim Bolton, Conference of the American Physical Society, March 2002.

19. 'A QM/MM study of HCl adsorption on ice surfaces', K. Bolton, 4th European Computational Chemistry Conference, Assisi, Italy, 1 September 2002.
20. 'Manipulation and separation of carbon nanotubes based on their chirality', Arne Rosén, Simon Gustavsson and Kim Bolton, Conference of the American Physical Society, Austin, Texas, March 3-7, 2003.
21. 'Simulation of water-polymer systems', E. Johansson, K. Bolton and P. Ahlström, Thermodynamics and Statistical Mechanics with Industrial Applications, University of Cambridge, U.K., 9-11 April 2003.
22. 'Manipulation and separation of carbon nanotubes based on their chirality', Kim Bolton, Arne Rosén and Simon Gustavsson, NT03, Seoul, Korea, 7 July 2003.
23. 'Manipulation and separation of carbon nanotubes based on their chirality', Arne Rosén, Simon Gustavsson and Kim Bolton, Third IEEE Conference on Nanotechnology, San Francisco, USA, August 12-14, 2003.
24. "Molecular Simulation of VLE for Mixtures of Hydrofluorocarbon Compounds Using a Modified Stockmayer Potential", T. J. McKnight, D. Ramjugernath, M Starzak and K Bolton, South African Institute for Chemical Engineering Congress, 3-5 September, 2003.
25. "Monte Carlo Simulation of Pure HCFC and HFC compounds using a modified Stockmayer Potential", T. J. McKnight, D. Ramjugernath, M Starzak and K Bolton, South African Institute for Chemical Engineering Congress, 3-5 September, 2003.
26. 'Comparing the experimental and simulation approaches for the prediction of vapour-liquid phase equilibrium', T. J. McKnight, R. A. Harris, D. Ramjugernath, J. D. Raal, M Starzak and K Bolton, South African Institute for Chemical Engineering Congress, 3-5 September, 2003.
27. "Simulating vapour liquid equilibrium for mixtures of methanol using an effective Stockmayer potential", T. J. McKnight, D. Ramjugernath, M Starzak and K. Bolton, South African Institute for Chemical Engineering Congress, 3-5 September, 2003.
28. 'Phase diagrams of water from computer simulations', Erik Johansson, Kim Bolton and Peter Ahlström, South African Institute for Chemical Engineering Congress, 3-5 September, 2003.
29. 'Iron-carbide cluster thermal dynamics for catalysed carbon nanotube growth' Ding Feng, Kim Bolton and Arne Rosén, AVS 50th international symposium, Baltimore, USA, November 2-7 2003.
30. 'Coalescence of Metal Clusters at Temperatures below the Melting Point', Ding Feng, Kim Bolton and Arne Rosén, International Symposium on Cluster and Nano-Assemblies: Physical and Biological Systems, Virginia, USA, November 10-13, 2003.
31. 'Water and polyethylene insulators in electric fields' Erik Johansson, Peter Ahlström and Kim Bolton, Svensk Teoretisk Kemi, Lund, Sweden, November 15-16, 2003.
32. 'Electronic structure theory methods for molecular dynamics simulations' Kim Bolton, Svensk Teoretisk Kemi, Lund, Sweden, November 15-16, 2003.
33. 'Molecular dynamics study of catalyzed carbon nanotube growth within the vapor-liquid-solid model' Feng Ding, Arne Rosén and Kim Bolton, Okazaki, Japan, December 12-16 2003.
34. 'Collision-induced resistivity of carbon nanotubes' Kim Bolton, Arne Rosén, Hugo Romero and Peter Eklund, IWEPNM 2004, Kirchberg, Austria, March 2004
35. 'Molecular Dynamics Simulation of Single-Walled Carbon Nanotube Growth' Feng Ding, Kim Bolton and Arne Rosén, IWEPNM 2004, Kirchberg Austria, March 2004.

36. **Invited** 'Direct dynamics and QM/MM methods for studying large chemical systems' Kim Bolton, Applied Molecular Modeling and Simulation, Parys, South Africa, April 2004.
37. 'Molecular simulation of binary vapour liquid equilibrium', T. J. McKnight, D. Ramjugernath, K. Bolton and M Starzak, AMMS, Parys, South Africa, April 2004.
38. 'Simulation of conjugated alkenes using transferable united atom force fields' Kim Bolton, Peter Ahlström, Tyrone J. McKnight and Deresh Ramjugernath, Cimtec, Italy, May 30 – June 4, 2004.
39. **Invited** 'Molecular dynamics simulations of single-walled carbon nanotube nucleation', Kim Bolton, Feng Ding, and Arne Rosén, NT04, Mexico, July 19-23 2004.
40. 'Collision-induced resistivity of carbon nanotubes' Kim Bolton, Arne Rosén, Hugo Romero and Peter Eklund, NT04, Mexico, July 19-23 2004.
41. 'Theoretical Study of Catalytic Growth Single-Walled Carbon' Feng Ding, Kim Bolton and Arne Rosén, AVS, Anaheim, California, Nov 14-19, 2004.
42. 'Nucleation and Growth Mechanism of Single-Walled Carbon Nanotubes on the Surface of the Catalyst Particle: Molecular Dynamics Study' Feng Ding, Kim Bolton and Arne Rosén, AVS, ISSPIC, China, Sept 5-10, 2004.
43. 'Simulation of water vapour clusters in direct equilibrium with liquid water' Erik Johansson, Kim Bolton, Peter Ahlström, Conference on Computational Physics 2004, Genoa, Italy, Sept. 01-04, 2004.
44. 'Simulation of water vapour clusters in direct equilibrium with liquid water', E Johansson, K Bolton and P Ahlström, CCP5 Annual Meeting 2004, Sheffield, 1-4 September, 2004.
45. **Invited** 'Molecular dynamics of catalyzed single-walled carbon nanotube nucleation' Kim Bolton, Feng Ding, and Arne Rosén, TMS, San Fransisco, Feb. 13-17, 2005.
46. 'Nucleation of single-walled carbon nanotubes on catalyst particles: MD and electronic structure calculations', Arne Rosén, Feng Ding and Kim Bolton, Symposium on size selected clusters, Brand, Austria, Feb. 27 – March 4, 2005.
47. 'Molecular Simulation Studies of Water Vapour Clustering under Equilibrium Conditions', E Johansson, K Bolton and P Ahlström, Thermodynamics 2005, Sesimbra, 5-8 April, 2005.
48. **Invited** 'Molecular dynamics Studies of Catalyzed Single-Walled Carbon Nanotube Nucleation and Growth' Kim Bolton, Feng Ding, and Arne Rosén, NASA/Rice Workshop on Nucleation and Growth of SWNTs, Texas, Apr. 08-12, 2005.
49. 'Growth mechanisms of carbon nanotubes for polymer composites', Kim Bolton, Feng Ding, and Arne Rosén, First International Symposium on Nanostructured and Functional Polymer-Based Materials and Composites', Dresden, April 24-27, 2005.
50. 'Simulation of water vapour clusters in direct equilibrium with liquid water', Erik Johansson, Kim Bolton, Peter Ahlström, International meeting on polymer modelling and its industrial applications, Borås, Sweden, 6-8 June, 2005.
51. 'Microscopic modelling of polymers and their interactions' Peter Ahlstrom, Kim Bolton and Mikael Skrifvars, 3rd Industrial Simulation Conference, Berlin, June 9-11, 2005.
52. 'Modeling of nucleation and growth of single-walled carbon nanotubes within the catalytic chemical vapor deposition method', Arne Rosén, Kim Bolton and Feng Ding, ICTF13/ACSIN8 Congress, Stockholm, June 19-23 2005.

53. 'Nucleation of single-walled carbon nanotubes on catalyst particles: MD and electronic structure calculations', Feng Ding, Arne Rosén and Kim Bolton, NT05, Gothenburg, June 26 – July 1 2005.
54. 'Simulations of vapor water clusters at vapor-liquid equilibrium', Erik Johansson, Peter Ahlström and Kim Bolton, Conference of the American Physical Society, Baltimore, USA, March 2006.
55. 'Modeling the Melting of Free and Supported Metal Clusters', Kim Bolton, Feng Ding- Haiming Duan, Arne Rosén, Avetik R. Harutyunyan, Toshio Tokune and Stefano Curtarolo, Conference of the American Physical Society, Baltimore, USA, March 2006.
56. 'Carbon nanotube – metal cluster bond strengths: implications for catalytic growth', Peter Larsson, Feng Ding, J. Andreas Larsson, Arne Rosén, Rajeev Ahuja and Kim Bolton, Conference of the American Physical Society, Baltimore, USA, March 2006.
57. 'Potential models for iron and oxide surfaces and interfaces', Aiqin Jiang, Neha Awasthi, Aleksey Kolmogorov, Kim Bolton, Avetik R. Harutyunyan, Toshio Tokune and Stefano Curtarolo, Conference of the American Physical Society, Baltimore, USA, March 2006.
58. 'Phase diagrams for Fe-C nanoparticles: A Molecular Dynamics Study', Neha Awasthi, Aiqin Jiang, Aleksey Kolmogorov, Kim Bolton, Avetik R. Harutyunyan, Toshio Tokune and Stefano Curtarolo, Conference of the American Physical Society, Baltimore, USA, March 2006.
59. 'Computer animations for internet-based chemistry laboratories', Kim Bolton, Marko Korpi, Michael Christie and Elisabeth Saalman, Netlearning conference, Ronneby, Sweden, May 2006.
60. 'Datoranimeringar för aktiv lärande av kemiska koncept', Elisabeth Saalman, Marko Korpi, Michael Christie, Cedric Linder and Kim Bolton, Netlearning conference, Ronneby, Sweden, May 2006.
61. 'Modeling the Melting of Metal and Metal-Carbide Clusters' Kim Bolton, Haiming Duan, Feng Ding, Arne Rosén, Avetik R. Harutyunyan, Toshio Tokune, Aiqin Jiang, Aleksey Kolmogorov, Neha Awasthi and Stefano Curtarolo, NT'06, Nagano, Japan, June 2006.
62. 'Atomistic simulations of polymer and water', Peter Ahlström, Erik Johansson and Kim Bolton, Workshop on State-of-the-Art in Scientific and Parallel Computing, Umeå, June, 2006.
63. 'Modeling the Melting Mechanism of Metal Clusters' Haiming Duan, Feng Ding, Arne Rosén, Avetik R. Harutyunyan, Elena Pigos, Toshio Tokune, Aleksey Kolmogorov, Stefano Curtarolo and Kim Bolton, ISSPIC XIII, Gothenburg, Sweden, July 2006.
64. 'Molecular Simulation of Carboxylic Acids', Scott Clifford, Deresh Ramjugernath and Kim Bolton, 19th International Conference on Chemical Thermodynamics, Boulder, Colorado, July 30-August 4, 2006.
65. 'Parameterization of H₂S, SO₂ and NO₂', Scott Clifford, Deresh Ramjugernath and Kim Bolton, 19th International Conference on Chemical Thermodynamics, Boulder, Colorado, July 30-August 4, 2006.
66. 'The effects of oxide substrates (Al₂O₃ and SiO₂) on phase diagrams for Fe-C nanoparticles. Ab initio and molecular dynamics studies.' Aiqin Jiang, Neha Awasthi, Aleksey Kolmogorov, Elena Mora, Toshio Tokune, Avetik R. Harutyunyan, Arne Rosén, Kim Bolton and Stefano Curtarolo, XV international materials research congress, Mexico, August 2006

67. 'Use of metal clusters in catalysis and for the growth of SWNT', Arne Rosen, Kim Bolton and Mats Andersson, ACS National Meeting, San Francisco, USA, September, 2006.
68. 'Carbon Nanotube - Metal Cluster Bond Strengths: Implications For Catalytic Growth', P. Larsson, F. Ding, J. A. Larsson, A. Rosén, R. Ahuja, K. Bolton, Diamond 2006, Estoril, Portugal, September, 2006.
69. **Invited** 'Modelling SWNT growth and properties', Kim Bolton and Arne Rosén, CECAM workshop Simulations novel carbon materials, Lyon, France, October 2006.
70. 'The Importance of Metal particle - Nanotube Binding for Single Walled Nanotube Growth', F. Ding, P. Larsson, R. Ahuja, J. A. Larsson, H. Duan, A. Rosen, K. Bolton, 11th Irish Atomistic Simulators Meeting, Belfast, Northern Ireland, December, 2006.
71. 'Distribution and stability of Carbon in Fe-C nanoparticles.', N. Awasthi, A. Jiang, A. Kolmogorov, W. Setyawan, K. Bolton and S. Curtarolo, Conference of the American Physical Society, USA, March 2007.
72. 'Challenges for Growth of Smallest Diameter Single-Walled Carbon Nanotubes by Catalytic Method', Oleg A. Kuznetsov, Elena Mora, Toshio Tokune, Stefano Curtarolo, Kim Bolton, and Avetik R. Harutyunyan, Meeting of the American Physical Society, USA, March 2007.
73. **Invited** 'Computational modeling of SWCNTs and their growth', Kim Bolton, NASA/Rice Workshop on Nucleation and Growth of SWNTs, Texas, Apr. 13-17, 2007.
74. 'Strong SWNT-catalyst adhesion strength as a necessary condition for SWNT growth', Feng Ding, Peter Larsson, J. Andreas Larsson, Rajeev Ahuja, Haiming Duan, Arne Rosén, Kim Bolton, The Electrochemical Society Meeting, Chicago, May 6-11 2007.
75. 'Molecular Simulation of solubilities and structure of water in n-alkanes and polyethylene', E. Johansson, K. Bolton, P. Ahlström and D.N. Theodorou, Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design, Hersonissos, 20-25 May, 2007.
76. 'Size effects on the stability of Carbon in Fe-C nanoparticles' Stefano Curtarolo, Neha Awasthi, Aiqin Jiang, Aleksey Kolmogorov, Wahyu Setyawan, Kim Bolton, Toshio Tokune, Elena Mora, Avetik R. Harutyunyan, E-MRS, France, May 28 2007.
77. 'On the Interfacial Interaction Between Nanocatalysts and Various Oxide Substrates' Gamini Sumanasekera, Kapila Hewaparakrama, Kim Bolton, Stefano Curtarolo, Avetik R. Harutyunyan, NT07, Brazil, June 23-29, 2007.
78. 'Strong SWNT-catalyst adhesion strength as a necessary condition for single-walled carbon nanotube growth', Feng Ding, Peter Larsson, J. Andreas Larsson, Rajeev Ahuja, Haiming Duan, Arne Rosén, Kim Bolton, Carbon 2007.
79. 'Diameter and Chirality Changes of Single-Walled Carbon Nanotubes During Growth: An ab-initio Study', Wuming Zhu, Haiming Duana, Arne Rosén and Kim Bolton, ChinaNANO 2007, June 2007, Beijing, China.
80. 'Modeling size- and thermodynamic stability- effects on Fe-C and Fe-Mo-C nanocatalysts.' Stefano Curtarolo, Neha Awasthi, Aiqin Jiang, Aleksey Kolmogorov, Wahyu Setyawan, Kim Bolton, Toshio Tokune, Elena Mora, Avetik R. Harutyunyan, NT'07, Brazil, June 2007.
81. **Invited** 'Carbon nanotube growth mechanisms', Kim Bolton, Diamond-2007, Berlin, September 10-14, 2007.
82. 'Carbon metal interactions and epitaxy in nanotube growth: Towards chirality-selected nanotube production', Feng Ding, Peter Larsson, Andreas Larsson, Rajeev

- Ahuja, Kim Bolton, Arne Rosen, Boris I Yakobson, Materials Research Society meeting, November 26 - 30, 2007.
83. 'The role of carbon solubility in Fe-C nano-clusters on the growth of small single-walled carbon nanotubes' Stefano Curtarolo, Neha Awasthi, Wahyu Setyawan, Elena Mora, Toshio Tokune, Kim Bolton, Avetik R. Harutyunyan, Meeting of the American Physical Society, USA, March 2008.
 84. 'The apparent paradox of the Gibbs-Thompson phenomenon is the thermodynamic limit for the activity of Fe and Fe:Mo catalysts for carbon nanotubes growth', Stefano Curtarolo, N. Awasthi, W. Setyawan, T. Tokune, E. Mora, O. Kuznetsov, A. Harutyunyan, Kim Bolton, NT08, Montpellier, June 28-July 3, 2008.
 85. 'Theoretical investigation of the Nanotube-metal junction', A. Börjesson, W. Zhu, H. Amara, C. Bichara, F. Ducastelle and K. Bolton, NT08, Montpellier, June 28-July 3, 2008.
 86. **Invited** 'Simulations of water, metal and carbon clustering' Kim Bolton, Workshop on Nucleation of inorganic atmospheric clusters and particles, Gothenburg, August 13-15, 2008.
 87. 'Computer Simulations of Vapor-Liquid-Liquid Equilibria Involving Hydrocarbons and Water', Suren Moodley, Peter Ahlström, Kim Bolton and D. Ramjugernath, AIChE Annual Meeting, Philadelphia, November 15-21, 2008.
 88. 'On Polyethylene Cable Failure, Electric Fields, Water Clusters and Ions', E. Johansson, K. Bolton and P. Ahlström, American Institute for Chemical Engineering, Philadelphia November 16-21, 2008.
 89. 'Determination of binding energies of platinum ions on functionalized activated carbons through density functional theory', H. Kasaini, J. Mphahlele and K. Bolton, *Minerals Engineering International Conference: Computational Modelling 08*, Cape Town, South Africa, November 13-14, 2008
 90. 'Modelling carbon nanotube growth', Kim Bolton, CHPC National Meeting, Durban, South Africa, December 9-10, 2008.
 91. 'Computer Simulations of Vapor-Liquid-Liquid Equilibria Involving Hydrocarbons and Water', Suren Moodley, Peter Ahlström, Kim Bolton and D. Ramjugernath, CHPC National Meeting, Durban, South Africa, December 9-10, 2008.
 92. 'Simulations of Water Clustering in Vapour, Hydrocarbons And Polymers' E. Johansson, K. Bolton and P. Ahlström, CHPC National Meeting, Durban, South Africa, December 9-10, 2008.
 93. **Invited** 'Computational studies of SWNT growth', Kim Bolton, NASA/Rice Workshop on Nucleation and Growth of SWNTs, Texas, Apr. 16-22, 2009.
 94. 'Modelling catalysed carbon nanotube growth', Kim Bolton, Materials Oriented Modelling – Catalysis and Interactions, Stockholm, June 28 – July 1, 2009.
 95. **Invited** 'Computational studies of single-walled carbon nanotube growth' Kim Bolton, International Symposium on Theory and Simulations of Complex Molecular Systems, Kyoto, Japan, July 19-21, 2009.
 96. 'Computer simulation studies of Carbon Nanotube – catalyst particle interfaces' Anders Börjesson, Hakim Amara, Kim Bolton and Christophe Bichara, MRS, San Francisco, USA, April 5-9, 2010.
 97. 'Continuum - Molecular Modeling of Graphene Lattice' K. Samadikhah, R. Larsson, K. Bolton, F. Bazooyar, IV European Conference on Computational Mechanics, Paris, France, May 16-21, 2010
 98. 'Water absorption in polymers', Peter Ahlström, Tobias Gebäck, Erik Johansson and Kim Bolton, European Conference on Computational Chemistry, Lund, Sweden, 25-28 August 2010.

99. 'Modelling of Carbonaceous Polymeric Nanocomposites', Kavitha Chelakara Satyanarayana, Shayesteh Haghghatpanah and Kim Bolton, European Conference on Computational Chemistry, Lund, Sweden, 25-28 August 2010.
100. **Invited**: 'Modelling of carbon nanotube growth', Anders Börjesson and Kim Bolton, NASA/Rice Workshop on Nucleation and Growth of SWNTs, Texas, Apr. 8-12, 2011.
101. 'Simulations of water solubility in polyethylene and cellulose', Kim Bolton, Erik Johansson, Faranak Bazooyar, Anders Börjesson and Peter Ahlström, Nordic Polymer Days 2011, Stockholm, Sweden, 15-17 June 2011.
102. 'Modelling of carbon nanotube polymer composites', Shayesteh Haghghatpanah, Martin Bohlén and Kim Bolton, Nordic Polymer Days 2011, Stockholm, Sweden, 15-17 June 2011.
103. 'Tailor-made materials from computer modeling' Anders Börjesson, Mikael Berlin, Thorbjörn Andersson, Peter Ahlström and Kim Bolton, Nordic Polymer Days 2011, Stockholm, Sweden, 15-17 June 2011.
104. 'Molecular Modeling of Systems Relevant to Cellulose Decomposition' Faranak Bazooyar and Kim Bolton, Nordic Polymer Days 2011, Stockholm, Sweden, 15-17 June 2011.
105. **Invited** 'Computational studies of single-walled carbon nanotube growth' Kim Bolton, Nano-S&T, Dalian, China, October 23-26, 2011.
106. 'Application of Molecular Mechanics and CSTR Experiments to Study Metal Adsorption by Oxalate-modified Activated Carbons' H. Kasaini, K. Bolton, P. Kekana, R. C. J. Mphahlele, 17th Symposium on Separation Science and Technology For Energy Application, Tennessee, USA, Oct 23 -27, 2011.
107. **Invited** 'Computational studies of single-walled carbon nanotube growth' Kim Bolton, Nanomaterials Conference, Puerto Morelos, Mexico, Nov. 28 – Dec 2, 2011.
108. 'Modelling of PVDF and PVDF-SWNT composites'. Kim Bolton, LefTex workshop, Gothenburg, Sweden, Dec. 8, 2011.
109. 'Computational studies on enhancing β -phase poly (vinylidene fluoride)', Kavitha Chelakara Satyanarayana, Martin Bohlén and Kim Bolton, SSF workshop on Functional Layers and Surfaces & Light Materials, Stockholm, Sweden, April 19 - 20 2012