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Editorial

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Editorial

Pacific Rim Conference on Nanoscience



The papers collected together in this special issue of *Molecular Simulation* were presented at the Broome nanoscience meeting in September 2004. They constitute a cross section of theoretical and experimental work related to nanomaterials and the behaviour of nanoscale systems. Such research creates the basis for more applied developments and for future nanotechnologies.

The Broome meeting was a unique opportunity for those of us working in nanoscience to spend five days discussing science with our colleagues from all over the world in a beautiful setting. I would like to thank the “local” committee from Curtin University in Perth, Gordon Parkinson, Julian Gale and Claire Hitchin, as well as the Conference and International committee, listed below. The conference was generously supported by the Western Australian government and the Perth Convention Bureau as well as Taylor & Francis, JEOL, and Accelrys. Thanks to Denis Evans for

suggesting the venue.

Nick Quirke
Imperial College

Broome Conference Committee

Prof. N. Quirke
Prof. G. Parkinson
Prof. D. Evans

International Advisory Committee

Prof. K.E. Gubbins
Prof. P. Cummings
Prof. A. Fuchs
Prof. K.Y. Chan
Prof. K. Kaneko
Prof. I. Snook
Prof. B. Todd
Prof. J. Schulte

Nanoscience - Broome

Programme

Tuesday, 7th September

13:45–14:00 Welcome to Broome: Conference aims and objectives
N. Quirke, Imperial College, London, UK

Session 1: Micro/nanofluidics—Chair: G. Parkinson

14:00–14:45 Nanofluidics
Thomas Becker, Universität Ulm, Ulm, Germany

14:45–15:30 Simulating Nanoflows
N. Quirke, Imperial College, London, UK

Session 2: Nanobio interfaces—Chair: N. Quirke

15:45–16:30 Ultramicroelectrodes for Detection of Chemical Messages
C. Amatore, Université de Paris, France

16:30–17:15 Poly-electrolytes at the Liquid Solid Interface: Biochips
M. Pettitt, University of Houston, USA

Conference Dinner—19:30 pool area

Wednesday, 8th September

Session 3: Nanofabrication I—Chair: D. Evans

08:30–09:15 Functional Interfaces and Nanostructures
T. Turney, CSIRO, University of Melbourne, Australia

09:15–10:00 Atomic-Scale Fabrication of a Silicon-based Quantum Computer
N. Curson, University of NSW, Australia

Session 4: Nanofabrication II—Chair: A. Fuchs

10:15–11:00 Nanoscale Writing and Imaging with Electron Beams
G. Rosolen, CSIRO, Australia

11:00–11:45 The Fluctuation Theorem, Theory and Experiment
D. Evans, Australian National University

Lunch Balcony area 12:00–13:30

Session 5: Water and aqueous solution—Chair: J. Gale

13:30–14:15 Electrolytes in Nanopores: Molecular Simulations and Related Applications
K. Y. Chan, University of Hong Kong, HK

14:15–14:45 Salinity and Energy: Challenges for Western Australia
J. Patroni, Department of the Premier and Cabinet, Western Australia

Session 6: Energy and minerals—Chair: K.Y. Chan

15:00–15:45 Nanoscience Opportunities
G. Parkinson, Curtin University, Australia

15:45–16:30 Designing Carbon Nanotubes for Energy Storage Applications
M. Lu, University of Queensland, Australia

16:30–17:15 Hydrogen Storage in Nanotubes—Has it all Gone Pear-shaped? A computational perspective
J. Gale, Curtin University, Australia

Thursday, 9th September

Session 7A: Hot Spot lectures—Chair: B. Todd

08:50–09:10 Theoretical Nanoscale Design of Self-Cleaning Surfaces
D. J. Henry, RMIT University, Australia

09:10–09:30 Computer Simulation of Electrodeposition—A Hybrid of Molecular Dynamics and Monte Carlo
Y. Kaneko, Y. Hiwatari and K. Ohara, Kyoto University, Japan

09:30–09:50 Interplay between Geometry and Interfacial Forces: New Mechanisms for Surface Activity of Nano-objects at Fluid–Fluid Interfaces
F. Bresme, Imperial College, UK

break

10:15–10:35 Aluminium Clusters for Hydrogen storage: a DFT Study
I. Yarovsky, RMIT University, Australia

10:35–10:55 Empirical Molecular Modelling of Crystal Growth Modifiers
F. Jones, NRI, Curtin University of Technology, Australia

10:55–11:15 DFT Studies of Surface Symmetry Dependence of SAMs on Gold Nanoparticles
C. Masens, University of Sydney, Australia

11:15–11:35 Structure of Gold Nanoclusters
B. J. Soule de Bas, University of Technology, Sydney, Australia

11:35–11:55 Strategic Partnership of Mitsubishi Corporation for Nanotechnology Business Creation
K. Shisbido, Mitsubishi Corporation

Lunch Balcony area 12:00– 13:30

Conference Tour

13:30–17:00 Trip to Willie Creek Pearl Farm, buses from reception

Session 8B: Poster Session and Hot Spot lectures—Chair: N. Quirke

19:20–19:40 Water Solvated Reaction System
D. L. Phillips, University of Hong Kong, HK

19:40–20:00 Statistical Mechanics of Fluids Adsorbed in Wedges and at Edges
J.R. Henderson, University of Leeds, UK

20:05–20:25 Computer Simulation of Carbon Nanotube Based Electric, Optical and Mechanical Devices
G. Chen, University of Hong Kong, HK

20:25–20:45 Viscous drag forces in gas operated pressure balances
V. Sokhan, Imperial College, UK

Followed by Posters in balcony area (drinks provided) until 23:00

Friday, 10th September

Session 8: Experimental nanosciences—Chair: P. Cummings

09:00–09:45 Compositionally Complex Colloidal Building Blocks
F. Caruso, University of Melbourne, Australia

09:45–10:30 Structural Anomalies of Classical Fluids, Quantum Fluids, and Solutions by Nanoconfinement
K. Kaneko, Chiba University, Japan

Session 9: Computational nanosciences—Chair: I. Snook

10:45–11:30 Computational and Theoretical Nanoscience: Essential Enabling Tools for Nanotechnology
P. Cummings, Vanderbilt University and Oak Ridge National Laboratory, USA

11:30–12:15 Nanostructure simulations
A. Fuchs, Universite de Paris Sud, France

Lunch Balcony area 12:30–14:30

14:30–15:15 On cats, maps and nanoflows: some recent developments in nonequilibrium nanofluidics
B. Todd, Swinburne, University of Technology, Melbourne

Session 10: Nanoparticles—Chair: N. Quirke

15:30–16:15 Nanostructured Nanoparticles: a new dimension in self-assembly
F. Stellacci, MIT, USA

16:15–17:00 Simulating Nanodiamonds
I. Snook, RMIT, Melbourne, Australia

17:00–17:10 Closing remarks
N. Quirke, Imperial College, London

Saturday, 11th September

Seminar on International Collaboration in Nanotechnology

09:30–09:40 Aims of Seminar
N. Quirke, Imperial College

09:40–10:00 Opportunities for collaboration through the Asia Pacific Nanotechnology Forum
J. Schulte, CEO APNF, Australia

10:00–10:30 EU Networks of Excellence/INSIDE PORES
N. Quirke, Imperial College

10:30–11:00 Collaboration through the Nanotechnology Consortium
A. Appleton, Accelrys

11:00–12:00 Coffee and general discussion