CURRICULUM VITAE

D. D. DO

PROFESSIONAL POSITIONS

Nov 91- present	Professor at University of Queensland
Nov 03 – Dec 03	Visiting Professor at Chiba University
Jan 86 - Nov 91	Associate Professor at University of Queensland
Aug - Sept 89	Visiting Professor at University of New Brunswick, Fredericton, CANADA
May - July 89	Visiting Scientist at ICI, Billingham, UNITED KINGDOM
July - Sept 87	Visiting Professor at Rensselaer Polytechnic Institute, Troy, NY, USA
Jan - Dec 85	Senior Lecturer at University of Queensland
July 81- Dec 84	Lecturer at University of Queensland
July 80 - June 81	Research Fellow at California Institute of Technology, Pasadena, California, USA
Jan - June 80	Senior Research Assistant at University of Queensland

UNIVERSITY EDUCATION

Degree:

B.E. (First Class Honours) University of Queensland, 1976
Ph.D. University of Queensland (April, 1980)

SCHOLARSHIPS, PRIZES

Colombo Plan Scholarship (1973-1976)
Dux of First Year (1973)
Union Carbide Prize (1976)
Commonwealth Research Award (1977-1979)
Esso award of Excellence in Chemical Engineering (1999)
Excellence in Teaching (2005)
Q-index Top 10 Researchers in University of Queensland (2011)
Fellow of the International Adsorption Society (IAS)

ORGANIZATION OF INTERNATIONAL CONFERENCE

Chairman and organiser, The Second Pacific Basin conference on Adsorption Science and Technology, May 14-18, 2000

EDITORIAL BOARD

Members of the editorial board of the following journals
1. Adsorption journal (1996 – present)
2. Adsorption Science & Technology (1997 – present)
3. Journal of non-equilibrium Thermodynamics (1999 – present)
4. Frontiers of Chemical Engineering in China (2006 – present)

CONFERENCE ORGANISATION

The Third Chemical Reaction Engineering Workshop, Brisbane, September 4-5, 1984, Chairperson.

The Second Pacific Basin Conference on Adsorption Science and Technology, Brisbane, May 14-18, 2000, Chairperson.

BOOKS

1- R. G. Rice and D. D. Do, "Applied Mathematics and Modeling for Chemical Engineers", Wiley & Sons, November 1994.
2- R. G. Rice and D. D. Do, "Solution manual for the Applied Mathematics and Modeling for Chemical Engineers", Wiley & Sons, July 1995.
3- D. D. Do, "Adsorption Analysis: Equilibria and Kinetics", Imperial College Press, London, 1998.
4- D. D. Do, "Adsorption Science and Technology", World Scientific Publishers, New Jersey, 2000.
5- R. G. Rice and D. D. Do, "Applied Mathematics and Modeling for Chemical Engineers", Second Edition, Wiley & Sons, September 2012.

PUBLICATIONS

2018

Adsorption on Nanopores of Different Cross Sections Made by Electron Beam Nanolithography, by Bruschi, Lorenzo; Mistura, Giampaolo; Prasetyo, Luisa; Do, Duong D.; Dipalo, Michele; De Angelis, Francesco From Langmuir (2018)	
An efficient kinetic Monte Carlo scheme for computing Helmholtz free energy and entropy in bulk fluids and adsorption systems, by Tan, Shiliang; Do, D. D.; Nicholson, D. From Chemical Engineering Journal (Amsterdam, Netherlands) (2018), 334, 1410-1421.	
Adsorption of argon on graphitized carbon black preloaded with methanol, ammonia and water: The role of adsorption regions and adsorbates, by Zeng, Yonghong; Xu, Hui; Do, D. D.; Nicholson, D. From Chemical Engineering Journal (Amsterdam, Netherlands) (2018), 334, 1316-1327	
A coherent definition of Henry constant and isosteric heat at zero loading for adsorption in solids - An absolute accessible volume By Prasetyo, Luisa; Do, D. D.; Nicholson, D. From Chemical Engineering Journal (Amsterdam, Netherlands) (2018), 334, 143-152	

2017

Development of averaged solid-fluid potential energies for layers and solids of various geometries and dimensionality, by Liu, Lumeng; Zeng, Yonghong; Do, D. D.; Nicholson, D.; Liu, Junjie From Adsorption (2017)	

Water adsorption on carbon - A review By Liu, Lumeng; Tan, Shiliang; Horikawa, Toshihide; Do, D. D.; Nicholson, D.; Liu, Junjie From Advances in Colloid and Interface Science (2017), 250, 64-78	
On the microscopic origin of the temperature evolution of isosteric heat for methane adsorption on graphite By Liu, Lumeng; Zhang, Han; Do, D. D.; Nicholson, D.; Liu, Junjie From Physical Chemistry Chemical Physics (2017), 19(39), 27105-27115	
Temperature dependence of water adsorption on highly graphitized carbon black and highly ordered mesoporous carbon, By Horikawa, Toshihide; Tan, Shiliang; Do, D. D.; Sotowa, Ken-ichiro; Alcantara-Avila, J. Rafael; Nicholson, D. From Carbon (2017), 124, 271-280.	DP16013540
Adsorption induced deformation in graphitic slit mesopores: A Monte Carlo simulation study By Diao, Rui; Fan, Chunyan; Do, D. D.; Nicholson, D. From Chemical Engineering Journal (Amsterdam, Netherlands) (2017), 328, 280-292	
On the evolution of the heat spike in the isosteric heat versus loading for argon adsorption on graphite-A new molecular model for graphite & reconciliation between experiment and computer simulation By Zeng, Yonghong; Horio, Keiji; Horikawa, Toshihide; Nakai, Kazuyuki; Do, D. D.; Nicholson, D. From Carbon (2017), 122, 622-634	
An improved model for N2 adsorption on graphitic adsorbents and graphitized thermal carbon black-The importance of the anisotropy of graphene By Prasetyo, Luisa; Tan, Shiliang; Zeng, Yonghong; Do, D. D.; Nicholson, D. From Journal of Chemical Physics (2017), 146(18), 184702/1-184702/14.	
Computational methodology for determining textural properties of simulated porous carbons By Phadungbut, Poomiwat; Herrera, L. F.; Do, D. D.; Tangsathitkulchai, Chaiyot; Nicholson, D.; Junpirom, Supunnee From Journal of Colloid and Interface Science (2017), 503, 28-38	
Adsorption of Methanol on highly graphitized thermal carbon black effects of the configuration of functional groups and their interspacing By Klomkliang, Nikom; Nantiphar, Orathai; Thakhat, Sarita; Horikawa, Toshihide; Nakashima, Kouki; Do, D. D.; Nicholson, D. From Carbon (2017), 118, 709-722	
On the consistency of NVT, NPT, μVT and Gibbs ensembles in the framework of kinetic Monte Carlo - Fluid phase equilibria and adsorption of pure component systems By Tan, Shiliang; Prasetyo, L.; Zeng, Y.; Do, D. D.; Nicholson, D. From Chemical Engineering Journal (Amsterdam, Netherlands) (2017), 316, 243-254. |	
A novel algorithm to accelerate the convergence of grand canonical Monte Carlo simulation of non-uniform fluids By Zeng, Yonghong; Do, D. D.; Nicholson, D. From Molecular Simulation (2017), 43(4), 243-249	
On the hysteresis of adsorption and desorption of simple gases in open end and closed end pores By Zeng, Yonghong; Prasetyo, Luisa; Tan, S. Johnathan; Fan, C.; Do, D. D.; Nicholson, D. From Chemical Engineering Science (2017), 158, 462-479	
A new kinetic Monte Carlo scheme with Gibbs ensemble to determine vapour-liquid equilibria By Tan, Shiliang Johnathan; Do, D. D.; Nicholson, D. From Molecular Simulation (2017), 43(2), 76-85	

On the resolution of constant isosteric heat of propylene adsorption on graphite in the sub-monolayer coverage region By Prasetyo, Luisa; Abdul Razak, Mus'ab; Do, D. D.; Horikawa, Toshihide; Nakai, Kazuyuki; Nicholson, D. From Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2017), 512, 101-110	
Adsorption of Ar and SO2 on graphitized carbon black: The importance of functional groups By Nickmand, Z.; Do, D. D.; Nicholson, D.; Aghamiri, S. F. From Adsorption (2017), 23(1), 57-62	

2016

Monte Carlo Simulation of Adsorption-Induced Deformation in Finite Graphitic Slit Pores Quick View Other Sources By Diao, Rui; Fan, Chunyan; Do, D. D.; Nicholson, D. From Journal of Physical Chemistry C (2016), 120(51), 29272-29282	
A GCMC simulation and experimental study of krypton adsorption/desorption hysteresis on a graphite surface By Prasetyo, Luisa; Horikawa, Toshihide; Phadungbut, Poomiwat; Tan, Shiliang; Do, D. D.; Nicholson, D. *Journal of Colloid and Interface Science* (2016), 478, 402-41.	DP16013540
Development of a grand canonical-kinetic Monte Carlo scheme for simulation of mixtures Tan, Shiliang; Do, D. D.; Nicholson, D. *Molecular Simulation* (2016), 42(12), 993-1000.	
On the adsorbate restructuring induced hysteresis of simple gas adsorption in slit micropores Diao, Rui; Fan, Chunyan; Do, D. D.; Nicholson, D. *Chemical Engineering Journal (Amsterdam*, Netherlands) (2016), 290, 381-390.	
Adsorption of water and methanol on highly graphitized thermal carbon black: The effects of functional group and temperature on the isosteric heat at low loadings Klomkliang, Nikom; Kaewmanee, R.; Saimoey, S.; Intarayothya, S.; Do, D. D.; Nicholson, D. *Carbon* (2016), 99, 361-369.	
On the explanation of hysteresis in the adsorption of ammonia on graphitized thermal carbon black By Zeng, Yonghong; Do, D. D.; Horikawa, Toshihide; Nicholson, D.; Nakai, Kazuyuki *Physical Chemistry Chemical Physics* (2016), 18(2), 1163-117.	

2015

Wedge Pore Model as an Alternative to the Uniform Slit Pore Model for the Determination of Pore Size Distribution in Activated Carbon By Zeng, Yonghong; Phadungbut, Poomiwat; Do, D. D.; Nicholson, D. *Journal of Physical Chemistry C* (2015), 119(46), 25853-25859.	
An efficient method to determine chemical potential of mixtures in the isothermal and isobaric bulk phase with kineticMonte Carlo simulation By Tan, Shiliang; Do, D. D.; Nicholson, D. *Molecular Physics* (2016), 114(2), 186-196.	

On the microscopic origin of the hysteresis loop in closed end pores - Adsorbate restructuring By Phadungbut, Poomiwat; Do, D. D.; Nicholson, D. *Chemical Engineering Journal* (Amsterdam, Netherlands) (2016), 285, 428-438.	
Application of kinetic Monte Carlo method to the vapour-liquid equilibria of associating fluids and their mixtures By Nguyen, Van T.; Tan, S. Johnathan; Do, D. D.; Nicholson, D. *Molecular Simulation* (2016), 42(8), 642-654.	
On the 2D-transition, hysteresis and thermodynamic equilibrium of Kr adsorption on a graphite surface By Diao, Rui; Fan, Chunyan; Do, D. D.; Nicholson, D. *Journal of Colloid and Interface Science* (2015), 460, 281-289.	
Hysteresis and scanning curves in linear arrays of mesopores with two cavities and three necks By Zeng, Yonghong; Tan, Shiliang Johnathan; Do, D. D.; Nicholson, D. *Colloids and Surfaces, A: Physicochemical and Engineering Aspects* (2016), 496, 52-62	
Adsorption of Water and Methanol on Highly Graphitized Thermal Carbon Black and Activated Carbon Fibre By Horikawa, Toshihide; Takenouchi, Masanori; Do, Duong D.; Sotowa, Ken-ichiro; Alcantara-Avila, J. Rafael; Nicholson, David *Australian Journal of Chemistry* (2015), 68(9), 1336-1341.	
Scanning curves of water adsorption on graphitized thermal carbon black and ordered mesoporous carbon By Horikawa, Toshihide; Muguruma, Takahiro; Do, D. D.; Sotowa, Ken-ichiro; Alcantara-Avila, J. Rafael *Carbon* (2015), 95, 137-143.	
Undulation Theory and Analysis of Capillary Condensation in Cylindrical and Spherical Pores By Phadungbut, Poomiwat; Do, D. D.; Nicholson, D. *Journal of Physical Chemistry C* (2015), 119(35), 20433-20445.	
Scanning curves in wedge pore with the wide end closed: Effects of temperature By Klomkliang, Nikom; Do, Duong D.; Nicholson, David *AIChE Journal* (2015), 61(11), 3936-3943.	
Determination of absolute adsorption for argon on flat surfaces under sub- and supercritical conditions By Phadungbut, Poomiwat; Fan, Chunyan; Do, D. D.; Nicholson, D.; Tangsathitkulchai, Chaiyot *Colloids and Surfaces, A: Physicochemical and Engineering Aspects* (2015), 480, 19-27.	
Adsorption on Ordered and Disordered Duplex Layers of Porous Anodic Alumina By Bruschi, Lorenzo; Mistura, Giampaolo; Phadungbut, Poomiwat; Do, D. D.; Nicholson, D.; Mayamei, Yashar; Lee, Woo *Langmuir* (2015), 31(17), 4895-4905.	
Hysteresis Loop and Scanning Curves for Argon Adsorbed in Mesopore Arrays Composed of Two Cavities and Three Necks By Klomkliang, Nikom; Do, D. D.; Nicholson, D. *Journal of Physical Chemistry C* (2015), 119(17), 9355-9363.	
Existence of Ultrafine Crevices and Functional Groups along the Edge Surfaces of Graphitized Thermal Carbon Black By Zeng, Yonghong; Do, D. D.; Nicholson, D. *Langmuir* (2015), 31(14), 4196-4204.	

Novel approach to the characterization of the pore structure and surface chemistry of porous carbon with Ar, N2, H2O and CH3OH adsorption By Fan, C.; Nguyen, V.; Zeng, Y.; Phadungbut, P.; Horikawa, Toshihide; Do, D. D.; Nicholson, D. *Microporous and Mesoporous Materials* (2015), 209, 79-89.	
On Adsorption Hysteresis in Closed-End Pores: Isotherm Reconstruction and Free Energy Analysis Via Flat-Histogram Monte Carlo Simulation D. W. Siderius, V. K. Shen and D. D. Do Presented at AIChE Meeting, Salt Lake City, USA, November 2015	
The interplay between molecular layering and clustering in adsorption of gases on graphitized thermal carbon black - Spill-over phenomenon and the important role of strong sites By Do, D. D.; Johnathan Tan, S. L.; Zeng, Yonghong; Fan, Chunyan; Nguyen, Van T.; Horikawa, Toshihide; Nicholson, D. *Journal of Colloid and Interface Science* (2015), 446, 98-113.	
On the phase transition of argon adsorption in an open end slit pore-Effects of temperature and pore size Phadungbut, Poomiwat; Do, D. D.; Nicholson, D.; Tangsathitkulchai, Chaiyot *Chemical Engineering Science* (2015), 126, 257-266.	
Adsorption in alumina pores open at one and at both ends By Bruschi, Lorenzo; Mistura, Giampaolo; Nguyen, Phuong T. M.; Do, Duong D.; Nicholson, David; Park, Sang-Joon; Lee, Woo *Nanoscale* (2015), 7(6), 2587-2596.	
On the isosteric heat of adsorption of non-polar and polar fluids on highly graphitized carbon black Horikawa, Toshihide; Zeng, Yonghong; Do, D. D.; Sotowa, Ken-Ichiro; Alcantara Avila, Jesus Rafael *Journal of Colloid and Interface Science* (2015), 439, 1-6.	
A molecular simulation study of adsorption and desorption in closed end slit pores: Is there a hysteresis loop? Fan, Chunyan; Zeng, Yonghong; Do, D. D.; Nicholson, D. *Chemical Engineering Science* (2015), 121, 313-321.	
Characterization of oxygen functional groups on carbon surfaces with water and methanol adsorption Zeng, Yonghong; Prasetyo, Luisa; Nguyen, Van T.; Horikawa, Toshihide; Do, D. D.; Nicholson, D. *Carbon* (2015), 81, 447-457.	
On the existence of a hysteresis loop in open and closed end pores Fan, Chunyan; Do, D. D.; Nicholson, D. *Molecular Simulation (2015), 41(4), 245-255.*	DP0987969

2014

Anatomy of Adsorption in Open-End and Closed-End Slit Mesopores: Adsorption, Desorption, and Equilibrium Branches of Hysteresis Loop Zeng, Yonghong; Phadungbut, Poomiwat; Do, D. D.; Nicholson, D. *Journal of Physical Chemistry C* (2014), 118(44), 25496-25504.	
Hysteresis Loop and Scanning Curves of Argon Adsorption in Closed-End Wedge Pores	

Klomkliang, Nikom; Do, D. D.; Nicholson, D. *Langmuir* (2014), 30(43), 12879-12887.	
On the phase transition in a monolayer adsorbed on graphite at temperatures below the 2D-critical temperature Phadungbut, Poomiwat; Nguyen, Van T.; Do, D. D.; Nicholson, D.; Tangsathitkulchai, Chaiyot *Molecular Simulation* (2014), Ahead of Print	
An undulation theory for condensation in open end slit pores. Critical hysteresis temperature & critical hysteresis pore size Fan, Chunyan; Zeng, Yonghong; Do, D. D.; Nicholson, D. *Physical Chemistry Chemical Physics* (2014), 16(24), 12362-12373.	
Evaporation from an Ink-Bottle Pore: Mechanisms of Adsorption and Desorption Zeng, Yonghong; Fan, Chunyan; Do, D. D.; Nicholson, D. *Industrial & Engineering Chemistry Research* (2014), 53(40), 15467-15474.	
Reconciliation of different simulation methods in the determination of the equilibrium branch for adsorption in pores Nguyen, Van T.; Do, D. D.; Nicholson, D. *Molecular Simulation* (2014), 40(7-9), 713-720.	
Condensation and Evaporation in Slit-Shaped Pores: Effects of Adsorbate Layer Structure and Temperature, Zeng, Yonghong; Fan, Chunyan; Do, D. D.; Nicholson, D. *Journal of Physical Chemistry C (2014), 118(6), 3172-3180.*	DP0987969
A comparative study of the adsorption of water and methanol in zeolite BEA: a molecular simulation study Nguyen, Van T.; Nguyen, Phuong T. M.; Dang, Liem X.; Mei, Donghai; Wick, Collin D.; Do, D. D. *Molecular Simulation* (2014), 40(14), 1113-1124.	DP0987969
Effects of temperature, pore dimensions and adsorbate on the transition from pore blocking to cavitation in an ink-bottle pore Klomkliang, Nikom; Do, D. D.; Nicholson, D. *Chemical Engineering Journal* (2014), 239, 274-283.	DP0987969
A new molecular model for water adsorption on graphitized carbon black Nguyen, Van T.; Do, D. D.; Nicholson, D. *Carbon* (2014), 66, 629-636.	DP0987969
Water as a potential molecular probe for functional groups on carbon surfaces Nguyen, Van T.; Horikawa, Toshihide; Do, D. D.; Nicholson, D. *Carbon* (2014), 67, 72-78.	DP0987969
Chemical potential, Helmholtz free energy and entropy of argon with kinetic Monte Carlo simulation Fan, C.; Do, D. D.; Nicholson, D.; Ustinov, E. *Molecular Physics* (2014), 112(1), 60-73.	DP0987969

2013

On the hysteresis loop and equilibrium transition in slit-shaped ink-bottle pores Klomkliang, Nikom; Do, D. D.; Nicholson, D. *Adsorption* (2013), 19(6), 1273-1290.	DP0987969

Development of kinetic Monte Carlo and Bin-Monte Carlo schemes for simulation of mixtures - vapor-liquid equilibria & adsorption Nguyen, Van T.; Fan, Chunyan; Abdul Razak, Mu'sab; Do, D. D.; Nicholson, D.; Ustinov, E. *Chemical Engineering Science* (2013), 102, 220-226.	DP0987969
Simulation study of two-dimensional phase transitions of argon on graphite surface and in slit micropores Ustinov, Eugene A.; Do, D. D. *Adsorption* (2013) 20, 439-451.	DP0987969
A Monte Carlo study of equilibrium transition in finite cylindrical pores Liu, Zhongjun; Nguyen, Van T.; Do, D. D.; Nicholson, D. *Molecular Simulation* (2013) 40, 966-975.	DP0987969
Condensation and Evaporation in Capillaries with Nonuniform Cross Sections Fan, Chunyan; Do, D. D.; Nicholson, D. *Industrial & Engineering Chemistry Research* (2013), 52(39), 14304-14314.	DP0987969
GCMC simulation of argon adsorption in wedge shaped mesopores of finite length Nickmand, Zahra; Do, D. D.; Nicholson, D.; Aghamiri, Seyed Foad; Khozanie, Mohammad Reza Talaie; Sabzyan, Hasan *Adsorption* (2013), 19(6), 1245-1252.	DP0987969
On the relative strength of adsorption of gases on carbon surfaces with functional groups: fluid-fluid, fluid-graphite and fluid-functional group interactions Nguyen, Van T.; Horikawa, Toshihide; Do, D. D.; Nicholson, D. *Carbon* (2013), 61, 551-557.	DP0987969
On the hysteresis of argon adsorption in a uniform closed end slit pore Fan, Chunyan; Do, D. D.; Nicholson, D. *Journal of Colloid and Interface Science* (2013), 405, 201-210.	DP0987969
Preparation of nitrogen-doped porous carbon and its water adsorption behaviour Horikawa, Toshihide; Sakao, Noriyuki; Hayashi, Jun-ichi; Do, D. D.; Katoh, Masahiro; Sotowa, Ken-ichiro *Adsorption Science & Technology* (2013), 31(2/3), 135-144.	DP0987969
Pore connectivity and hysteresis in gas adsorption: A simple three-pore model Nguyen, Phuong T. M.; Do, D. D.; Nicholson, D. *Colloids and Surfaces, A: Physicochemical and Engineering Aspects* (2013), 437, 56-68.	DP0987969
Effects of melting and ordering on the isosteric heat and monolayer density of argon adsorption on graphite Ustinov, Eugene A.; Do, Duong D. *Adsorption* (2013), 19(2-4), 291-304.	DP0987969
Microscopic configurations of methanol molecules in graphitic slit micropores. A computer simulation study Nguyen, Van T.; Do, D. D.; Nicholson, D. *Journal of Colloid and Interface Science* (2013), 396, 215-226.	DP0987969
On the Cavitation-Like Pore Blocking in Ink-Bottle Pore: Evolution of Hysteresis Loop with Neck Size Nguyen, Phuong T. M.; Fan, Chunyan; Do, D. D.; Nicholson, D. *Journal of Physical Chemistry C* (2013), 117(10), 5475-5484.	DP0987969
On the condensation/evaporation pressures and isosteric heats for argon adsorption in pores of different cross-sections Wang, Yao; Do, D. D.; Herrera, L. F.; Nicholson, D.	DP0987969

Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2013), 420, 96-102.	
On the Irreversibility of the Adsorption Isotherm in a Closed-End Pore Nguyen, Phuong T. M.; Do, D. D.; Nicholson, D. *Langmuir* (2013), 29(9), 2927-2934.	DP0987969
A novel application of kinetic Monte Carlo method in the description of N2 vapor-liquid equilibria and adsorption Fan, Chunyan; Do, D. D.; Nicholson, D.; Ustinov, E. *Chemical Engineering Science* (2013), 90, 161-169.	DP0987969
On the description of isotherms of CH4 and C2H4 adsorption on graphite from subcritical to supercritical conditions Abdul Razak, Mus'ab; Do, D. D.; Horikawa, Toshihide; Tsuji, Keita; Nicholson, D. *Adsorption* (2013), 19(1), 131-142.	DP0987969
Simulation study of hysteresis of argon adsorption in a conical pore and a constricted cylindrical pore Nguyen, Phuong T. M.; Do, D. D.; Nicholson, D. *Journal of Colloid and Interface Science* (2013), 396, 242-250.	DP0987969
Effects of temperature on water adsorption on controlled microporous and mesoporous carbonaceous solids Horikawa, Toshihide; Sakao, Noriyuki; Do, D. D. *Carbon* (2013), 56, 183-192.	DP0987969
Bin-Monte Carlo simulation of ethylene coexistence and of ethylene adsorption on graphite Fan, Chunyan; Do, D. D.; Nicholson, D. *Colloids and Surfaces, A: Physicochemical and Engineering Aspects* (2013), 437, 42-55.	DP0987969
On the hysteresis and equilibrium phase transition of argon and benzene adsorption in finite slit pores. Monte Carlo vs. Bin-Monte Carlo Klomkliang, Nikom; Do, D. D.; Nicholson, D. *Chemical Engineering Science* (2013), 87, 327-337.	DP0987969
Monte Carlo simulation and experimental studies on the low temperature characterization of nitrogen adsorption on graphite, Fan, Chunyan; Do, D. D.; Nicholson, D.; Jagiello, Jacek; Kenvin, Jeffrey; Puzan, Marissa, *Carbon* (2013), 52, 158-170	DP0987969

2012

Azeotropic adsorption equilibrium of mixed organic solvent on FAU type high silica zeolite - interpretation by molecular simulation and Do's method *Chihara, Kazuyuki; Taira, Tatsuharu; Yamada, Natsuki; Suzuki, Yusuke; Do, D. D.* AIChE Meeting, Conference Proceedings, Pittsburgh, PA, USA, Oct. 28-Nov. 2 (2012).	
Solid deformation induced by the adsorption of methane and methanol under sub- and supercritical conditions, Nguyen, Van T.; Do, D. D.; Nicholson, D. *Journal of Colloid and Interface Science* (2012), 388(1), 209-218	DP0987969
The effect of zeolite treatment by acids on sodium adsorption ratio of coal seam gas water, Wang, Xiaoyu; Ozdemir, Orhan; Hampton, Marc A.; Nguyen, Anh V.; Do, D. D. *Water Research* (2012), 46(16), 5247-5254	
Simulation of gas adsorption on a surface and in slit pores with grand canonical and	DP0987969

canonical kinetic Monte Carlo methods, Ustinov, E. A.; Do, D. D., *Physical Chemistry Chemical Physics* (2012), 14(31), 11112-11118	
Computer Simulation of Benzene-Water Mixture Adsorption in Graphitic Slit Pores, Nguyen, Phuong T. M.; Do, D. D.; Nicholson, D., *Journal of Physical Chemistry C* (2012), 116(26), 13954-13963	DP0987969
Thermodynamic Analysis of Ordered and Disordered Monolayer of Argon Adsorption on Graphite. Ustinov, Eugene A.; Do, D. D. *Langmuir,* (2012), 28(25), 9543-9553	DP0987969
A new and effective Bin-Monte Carlo scheme to study vapour-liquid equilibria and vapour-solid equilibria Fan, Chunyan; Do, D. D.; Nicholson, D. *Fluid Phase Equilibria* (2012), 325, 53-65	DP0987969
The concept of mean free path in the kinetic Monte Carlo description of bulk fluid behaviour, vapour-liquid equilibria and surface adsorption of argon Fan, Chunyan; Do, D. D.; Nicholson, D. *Molecular Simulation,* (2012), 38(12), 1001-1009	
Two-dimensional order-disorder transition of argon monolayer adsorbed on graphitized carbon black: Kinetic Monte Carlo method Ustinov, E. A.; Do, D. D. *Journal of Chemical Physics* (2012), 136(13), 134702/1-134702/10	
Application of the kinetic Monte Carlo method in the microscopic description of argon adsorption on graphite, Nguyen, Van T.; Do, D. D.; Nicholson, D.; Ustinov, E. A., *Molecular Physics*, (2012), 110(18), 2281-2294	
A computer simulation and experimental study of the difference between krypton adsorption on a graphite surface and in a graphitic hexagonal pore, Wang, Yao; Abdul Razak, Musab; Do, D. D.; Horikawa, Toshihide; Morishige, Kunimitsu; Nicholson, D., *Carbon* (2012), 50(8), 2908-2917	DP0987969
Affinity and Packing of Benzene, Toluene, and p-Xylene Adsorption on a Graphitic Surface and in Pores, Klomkliang, Nikom; Do, D. D.; Nicholson, D., *Industrial & Engineering Chemistry Research* (2012), 51(14), 5320-5329	DP0987969
Preparation of nitrogen-doped porous carbon by ammonia gas treatment and the effects of N-doping on water adsorption, Horikawa, Toshihide; Sakao, Noriyuki; Sekida, Tomoki; Hayashi, Jun-ichi; Do, D. D.; Katoh, Masahiro, *Carbon* (2012), 50(5), 1833-1842	DP0987969
A thermodynamic study of the mid-density scheme to determine the equilibrium phase transition in cylindrical pores, Liu, Zhongjun; Do, D. D.; Nicholson, D., *Molecular Simulation* (2012), 38(3), 189-199	DP0987969
Packing effects on argon and methanol adsorption inside graphitic cylindrical and slit pores: A GCMC simulation study, Liu, Zhongjun; Horikawa, Toshihide; Do, D. D.; Nicholson, D., *Journal of Colloid and Interface Science* (2012), 368(1), 474-487	DP0987969

Multilayer adsorption of benzene on graphitised thermal carbon black. The importance of quadrupole and explicit hydrogen in the potential model, Klomkliang, Nikom; Do, D. D.; Nicholson, D.; Tangsathitkulchai, C.; Wongkoblap, A. *Chemical Engineering Science* (2012), 69(1), 472-482	
On the Identification of the Sharp Spike in the Heat Curve for Argon, Nitrogen, and Methane Adsorption on Graphite: Reconciliation between Computer Simulation and Experiments, Fan, Chunyan; Razak, Musab Abdul; Do, D. D.; Nicholson, D., *Journal of Physical Chemistry C* (2012), 116(1), 953-962	
Application of kinetic Monte Carlo method to equilibrium systems: Vapour-liquid equilibria Ustinov, E. A.; Do, D. D., *Journal of Colloid and Interface Science* (2012), 366(1), 216-223	DP0987969
A self-consistent method to determine accessible volume, area and pore size distribution (APSD) of BPL, Norit and AX-21 activated carbon, Herrera, L. F.; Fan, Chunyan; Nguyen, Van; Do, D. D.; Horikawa, T.; Nicholson, D., *Carbon* (2012), 50(2), 500-509	DP0987969

2011

A revisit to the Gibbs dividing surfaces and helium adsorption, Herrera, L.; Fan, Chunyan; Do, D. D.; Nicholson, D., *Adsorption* (2011), 17(6), 955-965	
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