David Dubbeldam

Curriculum Vitae

Contact

University of Amsterdam,
Van 't Hoff Institute for Molecular Sciences, Faculty of Science,
Science Park 904, 1098 XH, Amsterdam, Noord-Holland,

Date of birth: 10-02-1971

Phone: +31 20 525 5054

ORCHID iD: 0000-0002-4382-1509

Researcher ID: B-6753-2014

D.Dubbeldam@uva.nl

http://www.uva.nl/profiel/d/u/d.dubbeldam/d.dubbeldam.html

1 Personal details

Bio

David Dubbeldam received a BSE and PhD from the University of Amsterdam, in computer science and computational chemistry, respectively. He completed his graduate work under the direction of Prof. Dr. Ir. B. Smit and worked with Prof. R.Q. Snurr during his post-doctoral study. Currently, he works as associate professor and VIDI laureate at the University of Amsterdam in the computational chemistry group. In 2011, he received the prestigious NWO VIDI grant (1 million euros) for a 5 year period to start up a group working on design and modeling of metal-organic frameworks. His group has developed the simulation code *RASPA* (a Monte-Carlo, Molecular Dynamics, and optimization code) and the macOS visualization app *iRASPA*.

Education

Ph.D., Computer Science with honor (cum laude), 28 October 2005
University of Amsterdam, Amsterdam, Noord-Holland
Thesis: *Computer-simulation of adsorption and diffusion of hydrocarbons in zeolites*
Adviser: Prof. Dr. Ir. B. Smit
Committee: Prof. dr. W. J. Briels, Prof. dr. D. Frenkel, Prof. dr. J. Kärger, Prof. dr. R. Krishna, Prof. dr. D. N. Theodorou, Prof. dr. J. M. Verstraten

M.S., Computer Science, 15 December 1997
University of Amsterdam, Amsterdam, Noord-Holland
Thesis: *Lattice Boltzmann simulation of fluid flow in a counterflow centrifugal elutriation chamber*
Adviser: Prof. P. Sloot

Employment

7/2019–present	Associate Professor (permanent position, 1.0 fte)
1/2010–7/2019	Assistant Professor (permanent position, 1.0 fte) Computational Chemistry Group, University of Amsterdam

1/2014–1/2019	Assistant Professor Delft (0.0 fte)
1/2011–1/2016	VIDI laureate
2/2009–12/2010	Post-doctoral research, Advisor: Prof. R. Krishna (fixed term, 1.0 fte) Computational Chemistry Group, University of Amsterdam Amsterdam, The Netherlands
2/2006–12/2008	Post-doctoral research, Advisor: Prof. R.Q Snurr (fixed term, 1.0 fte) Northwestern University, Evanston (IL), USA
1/2005–9/2005	Post-doctoral research (fixed term, 1.0 fte) CECAM Lyon, France
12/2000–12/2004	Ph.D research, Advisor: Prof. Dr. Ir. B. Smit (fixed term, 1.0 fte) ITS (Instituut voor Technische Scheikunde) at the University of Amsterdam
1/1998–8/2000	Scientific assistent ("wetenschappelijk medewerker", fixed term, 1.0 fte) group of Prof. P.M.A. Sloot at the University of Amsterdam

2 Research

Research focus

My research focuses broadly on the design and modeling of next-generation multifunctional, porous materials with molecule-specific properties for adsorption applications. Target applications include adsorption separations, air purification, carbon dioxide capture, energy storage, chemical sensing, and catalysis. I focus on developing new improved materials but also on elucidating the physical processes at the molecular level. Force field and method development are important aspects to make the simulations efficient, reliable, and predictive.

Selected invited visiting scientist

7 - 17 July 2018	Host: Prof. Randall Q. Snurr, Faculty Director, Chair of Chemical and Biological Engineering, Northwestern University, Evanston, USA.
16-20 oct 2014	Host: Prof. K.S. Walton, School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA.
7 - 15 Aug 2013	Host: Chris Wilmer, NuMat Technologies (`https://www.numat-tech.com`), Skokie, USA, and Prof. Randall Q. Snurr, Northwestern University, Evanston, USA.
1 - 30 Apr 2012	Host: Prof. W. Zhu, Full professor and director, Institute of Physical Chemistry, Zhejiang Normal University, P. R. of China.
22 - 29 Oct 2010	Host: Prof. K.S. Walton, School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA.
3 - 24 May 2010	Host: Dr. Anita Hill, Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia, Melbourne, Materials Science and Engineering.

Acting host at the UvA of short-term scientific visitors

1 July 2019	Prof. Dr. Vitaly Gitis (via a HRSMC fellowship joint application of Gadi Rothenberg, David Dubbeldam and Evert Jan Meijer), Ben Gurion University of the Negev, Israel, 3 months.
6 Nov 2017	Prof. Dr. J. Will Medlin (via a HRSMC fellowship joint application of Gadi Rothenberg and David Dubbeldam), University of Colorado, USA, 4 months.
1 May 2016	Phd student Salvador Rodriguez Gomez, Universidad Pablo de Olavide (Seville, Spain), 2 months.
25 April 2016	Prof. Dr. Krista Walton, School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA, 1 week.
1 Febr. 2016	Post-doc Federico Franco (via a HRSMC fellowship joint application of Jarl van der Vlugt, David Dubbeldam, and Stefania Grecea), University of Turin, Department of Chemistry, Italy, 6 months.
1 June 2015	Phd student Nicholas Burtch (via a GROW grant jointly applied with David Dubbeldam), School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA, 3 months.
1 May 2014	Phd student Salvador Rodriguez Gomez, Universidad Pablo de Olavide (Seville, Spain), 3 months.
1 June 2014	Phd student Nicholas Burtch (via a GROW grant jointly applied with David Dubbeldam), School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA, 3 months.
1 July 2013	Phd student Nicholas Burtch, School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA, 1 month.
9 Dec. 2012	Prof. Dr. Weidong Zhu, Full professor and director, Institute of Physical Chemistry,
1 July 2012	Phd student Juan José Gutiérrez Sevillano, Universidad Pablo de Olavide (Seville, Spain), 2 months.
1 July 2012	Phd student Nicholas Burtch, School of Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, USA, 2 months.
1 July 2011	Phd student Juan José Gutiérrez Sevillano, Universidad Pablo de Olavide (Seville, Spain), 2 months.
1 June 2010	Phd student Juan José Gutiérrez Sevillano, Universidad Pablo de Olavide (Seville, Spain), 3 months. Zhejiang Normal University, P. R. of China, 1 week.

PhD committees

16 April 2020	Seyed Hossein Jamali (prof. dr. T.J.H. Vlugt), "Transport Properties of Fluids: Methodology and Force Field Improvement using Molecular Dynamics Simulations", TU Delft.
14 April 2020	Nitish Govindarajan (prof. dr. E.J. Meijer), "Modeling Solvent Effects in Catalytic Reactions for Energy Conversion", University of Amsterdam.
18 Sept. 2019	Yiwen Tang (Dr. Stefania Grecea), "Metal-organic frameworks and their composites for water-alcohol separation applications", University of Amsterdam.
8 May 2019	Steven Vandenbrande (prof. dr. V. Van Speybroeck), Faculty of Engineering, Gent University, Belgium.

23 Sept. 2016	Alexandr Kachko (prof. dr. ir. T.J.H. Vlugt), "In-line monitoring of solvents during CO_2 absorption using multivariate data analysis", TU Delft.
19 April 2016	Nicholas Craig Burtch (prof. dr. K.S. Walton), "Developing Chemically Stable Metal-Organic Frameworks for Clean Energy technologies", Georgia Tech, Atlanta, USA.
5 febr. 2016	Bernardo Oyarzün (prof. dr. T.J.H. Vlugt), "molecular simulation of Liquid Crystals: Phase Equilibrium and the Solubility of Gases in Ordered Fluids", TU Delft.
5 Dec. 2015	Katya Davudova (prof. dr. ir. P.J. Schoenmakers), "Optimization of Designs for Spatial Multi-dimensional Separations", University of Amsterdam
4 June 2014	Evert Koopman (prof. dr. P.G. Bolhuis, dr. C.P. Lowe), "Simple numerical techniques for mesoscale polymers", University of Amsterdam.
1 Nov. 2013	Sondre Kvalvag Schnell (prof. dr. T.J.H. Vlugt), "Molecular Simulations of Zeolites: Heterogeneous Systems at Equilibrium and Non-Equilibrium: A Computational Study", TU Delft.
30 Oct. 2013	Anna Pavlova (prof. dr. E.J. Meijer), "Understanding the Role of Aqueous Solution in Chemical Reactions, University of Amsterdam.

PhD external committees

Jan. 2019	Abhishek Sharma, "Computational analysis of nonporous materials for gas adsorption and separation application", joint PhD program between IIT Bombay, India and Monash University, Australia.
Jan. 2018	José Manuel Vicent Luna, "Molecular Simulation of Ionic Liquids-Based Systems For Energy Applications", Universidad Pablo de Olavide (Seville, Spain).
Nov. 2011	Almudena García Sánchez, "Computational Study of Adsorption and Diffusion in Zeolites with Cations", Universidad Pablo de Olavide (Seville, Spain).
May. 2010	Elena Garciá Pérez, "Transport and Accessiblity in Zeolites and Metal-Organic Frameworks", Universidad Pablo de Olavide (Seville, Spain).

Selected invited lectures

4-6 June 2020	Erasmus Mundus Master 'Chemical Nanoengineering', Wroclaw University of Science and Technology, Wroclaw, Poland.
13 May 2020	UCL Chemical Engineering, University College London.
5 June 2019	CECAM workshop by Dmytro Antypov on "Accelerating material discovery by smart high-throughput computations", Materials Innovation Factory, Liverpool (UK).
18 Oct. 2017	"iRASPA: Computing Structure Properties of Nanoporous Materials on the GPU", Seminar University Pablo de Olavide, Seville, Spain.
6 Oct. 2015	"Exploiting Large-Pore Metal-Organic Frameworks for Separations using Entropic Molecular Mechanisms", Seminar Shell Amsterdam Noord.
27 March 2015	"Separating Xylene Isomers using Nanoporous Materials", Shell Amsterdam.
7 July 2014	"Understanding Zeolite Catalysis of Selective Hydroisomerization and Hydrocracking", Shell Amsterdam.
26-27 Oct. 2014	Gas Processing Conference (GPC), accepted paper "CO2/CH4 Solubility and Selectivity in Ionic Liquids", Mohammed Jaber F. Al Marri and Fadwa El Jack (Editors), Proceedings of the 4th International Gas Processing Conference, Doha, Qatar.

19 Aug 2013	”Computer-Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separation of Alkane isomers”, seminar at Department of Chemical and Biological Engineering, Northwestern University, Evanston, USA.
2-4 April 2013	”Computer-Assisted Screening of Ordered Crystalline Nanoporous Adsorbents for Separations of Alkane Isomers”, 16th and final Workshop of the International Research Training Group ”Diffusion in Porous Materials”.
6 April 2012	”Enantioselective Adsorption in A-Chiral Zeolites”, Zhejiang Normal University, Jinhua, P. R. of China.
13-15 May 2010	Panellist and invited speaker at the CSIRO Experimentalists and Molecular Modellers Conference, Clayton, Australia.
23 March 2009	”Metal-Organic Frameworks: Material Properties and Separation Applications”, Catalysts, Adsorbents and Colloids for Industry and Environemnt (ID09) and IAP Doctorate School, K.U. Leuven, Belgium.

Selected major collaborations

GTECH, USA	Long term collaboration since 2009 with the group of Prof. K.S. Walton, School of Chemical & Biomolecular Engineering, Georgia Institute of technology, USA. We have 1 joined book-chapter, 1 joined review article, and 5 joined peer-reviewed articles. Topic: water-stability of MOFs and experimental validation of simulation results.
Delft University	Long-term collaboration with the group of Prof. T.J.H Vlugt, Process & Energy Laboratory, Delft University of Technology, The Netherlands. We have 3 joined PhD students, and the collaboration has so far lead to more than 20 shared papers on topics such as simulations of ionic liquids, adsorption and diffusion in MOFs and zeolites, and development of statistical mechanical theory and new simulation methodology.
Seville, Spain	Long-term collaboration with the group of Prof. S. Calero, Physical Chemistry Division, University Pablo de Olavide, Spain. We have currently 1 shared PhD student, and more than 20 shared papers. Topic: computational modelling of zeolites and MOFs and software development.
HIMS	Long-term collaboration within HIMS with the group of Stefania Tanase Grecea from the group Heterogeneous Catalysis and Sustainable Chemistry. Topics include development of novel materials that could enable efficient adsorptive separations, for example, on-purpose design of new materials for separating saturated, unsaturated and aromatic hydrocarbon mixtures and seperating CO_2 from other gases. The collaboration has led to 1 joined paper published and one submitted.
ACMM	Collaboration within the Amsterdam Center of Multiscale Modeling (ACMM). ACMM is a center for theory and multiscale modeling in chemistry, physics and biology, which core is formed by the following three research groups: (1) Division of Theoretical Chemistry, VU University Amsterdam, (2) Computational Chemistry and Physics, University of Amsterdam, (3) FOM Institute for Atomic and Molecular Physics. Recent collaboration with Prof. C. Fonseca Guerra from the VU has lead to 1 joined article (more on the way). Topic: Quantum study and simulations of open-metal sites in MOFs.

Honors/Awards (main applicant)

2011	*NWO VIDI Grant 700.10.428*, 1 million euros

Earning power

2016 – present	Contribution to an awarded NWO Top-PUNT proposal, 2015, with various experimen-

tal HIMS colleagues G. Rothenberg, S. Grecea, J.I. van der Vlugt, D. Dubbeldam, J. van Maarseveen, J. Reek, B. de Bruin, and B. Feringa, sub-project 1 Phd student (Ilse Denekamp).

2016 – present joined application together with Prof. T.J.H Vlugt, proposal to Shell Amsterdam "Understanding adsorption, diffusion, and catalysis of aromatics in zeolites", 359k euros, 1 PhD as co-promotor (Sebastian Caro Ortiz).

2014 – present joined application together with Prof. T.J.H Vlugt, proposal to Shell Amsterdam "Understanding zeolite catalysis of selective hydro-isomerization and hydrocracking", 507k euros, 2 PhDs as co-promotor (Ali Poursaidesfahani and Tim Becker).

2015 GROW grant "Understanding and Increasing Water Stability in Metal-Organic Frameworks" visiting scientist Nicholas Burtch 040.15.020 (summer 2015).

2014 GROW grant "Mechanistic Insight into Structural Factors Governing Chemical Stability in Metal-Organic Frameworks" visiting scientist Nicholas Burtch 040.15.009 (summer 2014).

2013 – 2015 Open access grants, 036.002.508, 036.003.507, and 036.003.526.

2012 – 2014 KNAW "Samenwerkingsproject met China" (33k euros)

2011 – 2016 NWO VIDI personal grant 700.10.428, 1 million euros (NWO 800k euros, additional bonus of 200k by the University of Amsterdam).

2012 Ensing, Meijer, Dubbeldam, Molsim2012, CECAM Grant

2011 Ensing, Meijer, Dubbeldam, Molsim2011, ESF & CECAM Grant

External Reviewer

Chemistry: *J. Am. Chem. Soc., Angew. Chem. Int. Edit, J. Phys. Chem. B/C, Nature Chem., Nature Mat., Nano*,

Physics: *Phys. Rev, Lett., Phys. Rev. B, J. Chem. Phys.*

Citation analysis

google scholar:

	All	since 2015
Citations	7001	3592
h-index	44	29
h10-index	98	83

Bookchapters

D. Dubbeldam, S. Calero, T.J.H. Vlugt, and R.Q. Snurr, Chapter 5, "Simulations of Crystalline Nanoporous Materials", In: Dr. Vitaly Gitis and Gadi Rothenberger editors, "Handbook Vol. 1 - Synthesis, Characterization and Simulation of Porous materials", WorldScientific, 2020.

D. Dubbeldam. "Simulation of Crystalline Nanoporous Materials and the Computation of Adsorption/Diffusion Properties". In: T. Grant Glover and Bin Mu, editors, Gas Separations and Storage in Metal Organic Frameworks. CRC/Taylor & Francis, 2018.

D. Dubbeldam and K.S. Walton. "On the application of classical molecular simulations of adsorption in metal-organic frameworks". In Jiang Jianwen, editor, Metal-Organic Frameworks: Materials Modeling towards Engineering Applications. Pan Stanford Publishing Pte Ltd, 2015.

R.Q. Snurr, A.Ö. Yazaydin, D. Dubbeldam, and H. Frost. "Molecular modeling of adsorption and diffusion in metal-organic frameworks". In L.R. MacGillivray, editor, Metal-organic frameworks: design and application, Hoboken, NJ, 2010. Wiley.

Review articles

D. Dubbeldam, K.S. Walton, T.J.H. Vlugt, and S. Calero, Review: Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials, *Adv. Theory Simulat.*, 2019.

D. Dubbeldam, J. Vreede, S. Calero, and T.J.H. Vlugt, Review: Highlights of (Bio-)Chemical Tools and Visualization Software for Computational Science, *Current Opinion in Chemical Engineering*, 23, 1-13, 2019.

J. Heinen and D. Dubbeldam, Review: On flexible force fields for metal-organic frameworks: recent developments and future prospects, *WIREs Comput. Mol. Sci.*, 8.4, e1363, 2018.

A. Torres-Knoop and D. Dubbeldam, Review: Exploiting Large-Pore Metal-Organic Frameworks for Separations using Entropic Molecular Mechanisms, *Chem. Phys. Chem.*, 16(1), 2046-2067, 2015

D. Dubbeldam, S. Calero, and T.J.H. Vlugt, Review: Exploring New Methods and Materials for Enantioselective Separations and Catalysis *Mol. Simulat.*, 40(7-9), 585-598 (2014).

D. Dubbeldam, A. Torres-Knoop, and K.S Walton. Review: On the inner workings of monte carlo codes. *Mol. Simulat.*, 39(14), 1253-1292, 2013.

D. Dubbeldam and R.Q. Snurr. Review: Recent developments in the molecular modeling of diffusion in nanoporous materials. *Mol. Simulat.*, 33(4-5), 305-325, 2007.

Patent applications

"Process for separating mixtures containing straight-chain and branched alkanes" inventors: David Dubbeldam and Rajamani Krishna, Filed by Universiteit van Amsterdam, 27 April 2012 European Patent Office, Application No./12165907.2-2103

Publications (peer-reviewed)

132 journal papers, total times cited: 7001, google scholar: h-index 44, i10-index 98, top-5 best cited: 515, 497, 342, 301, 238, web of knowledge: h-index: 39

[132] R. Hens, A. Rahbari, S. Caro-Ortiz, N. Dawass, M. Erdos, A. Poursaeidesfahani, H. Salehi, A. Celebi, M. Ramdin, O. Moultos, D. Dubbeldam, and T.J.H. Vlugt. "Brick-CFCMC: open source software for Monte Carlo simulations of phase and reaction equilibria using the Continuous Fractional Component method." In: *J. Chem. Inf Model.* accepted (2020).

[132] A. Rahbari, R. Hens, O. Moultos, D. Dubbeldam, and T.J.H Vlugt. "Multiple free energy calculations from single state point Continuous Fractional Component Monte Carlo simulation using umbrella sampling." In: *J. Chem. Theory Comput.* 16.3 (2020), pp. 1757–1767.

[131] N. C. Burtch, I. M. Walton, J. T. Hungerford, C. R. Morelock, Y. Jiao, J. Heinen, Y.-S. Chen, A. A. Yakovenko, D. Dubbeldam W. Xu, and K. S. Walton. "In situ visualization of loading-dependent water effects in a stable metal-organic framework." In: *Nat. Chem.* 11.1-7 (2019), pp. 186–192.

[130] N.C. Burtch, S.J. Baxter, J. Heinen, A. Bird, A. Schneemann, D. Dubbeldam, and A. Wilkinson. "Negative Thermal Expansion Design Strategies in a Diverse Series of Metal-Organic Frameworks." In: *Adv. Func. Mater.* 30.37 (2019), p. 1704124.

[129] D. Dubbeldam, J. Vreede, T J.H. Vlugt, and S. Calero. "Highlights of (Bio-)Chemical Tools and Visualization Software for Computational Science." In: *Current Opinion in Chemical Engineering* 23 (2019), pp. 1–13.

[128] D. Dubbeldam, K.S. Walton, T.J.H. Vlugt, and S. Calero. "Design, Parameterization, and Implementation of Atomic Force Fields for Adsorption in Nanoporous Materials." In: *Adv. Theory Simulat.* 2.11 (2019), p. 1900135.

[127] A. Martin-Calvo, J.J. Gutierrez-Sevillano, D. Dubbeldam, and S. Calero. "Using aliphatic alcohols to tune benzene adsorption." In: *Adv. Theory Simulat.* 2.11 (2019), p. 1900112.

[126] I. Matito-Martos, J. García-Reyes, A. Martin-Calvo, D. Dubbeldam, and S. Calero. "Improving Ammonia Production Using Zeolites." In: *J. Phys. Chem. C* 123.30 (2019), pp. 18475–18481.

[125] S.C. Ortiz, R. Hens, E. Zuidema, M. Rigguto, D. Dubbeldam, and T J.H. Vlugt. "Molecular Simulation of the Vapor-Liquid Equilibria of Xylene mixtures: Force Field performance, and Wolf vs. Ewald for Electrostatic Interactions." In: *Fluid Phase Equilbria* 485.15 (2019), pp. 239–247.

[124] A. Poursaeidesfahani, E. Andres-Garcia, M. de Lange, A. Torres-Knoop, M. Rigutto, N. Nair, F. Kapteijn, J. Gascon, D. Dubbeldam, and T J.H. Vlugt. "Prediction of adsorption isotherms from breakthrough curves." In: *Micropor. Mesopor. Mater.* 277.15 (2019), pp. 237–244.

[123] A. Rahbari, R. Hens, D. Dubbeldam, and T.J.H. Vlugt. "Improving the accuracy of computing chemical potentials in CFCMC simulations." In: *Mol. Phys* 117.23/24 (2019), pp. 3493–3508.

[122] A. Rahbari, R. Hens, S.H. Jamali, M. Ramdin, D. Dubbeldam, and T J.H. Vlugt. "Effect of truncating electrostatic interactions on predicting thermodynamic properties of water-methanol systems." In: *Mol. Simulat.* 45.4/5 (2019), pp. 336–350.

[121] Y. Tang, D. Dubbeldam, X. Guo, G. Rothenberg, and S. Tanase. "Efficient separation of ethanol-methanol and ethanol-water mixtures using ZIF-8 supported on a hierarchical porous mixed-oxide substrate." In: *ACS Appl. Mater. Interfaces* 11.23 (2019), pp. 21126–21136.

[120] Y. Tang, D. Dubbeldam, and S. Tanase. "Water-ethanol and methanol-ethanol separations using in situ confined polymer chains in a metal-organic framework." In: *ACS Appl. Mater. Interfaces.* 11.44 (2019), pp. 41383–41393.

[119] T. Becker, L.-C. Lin, D. Dubbeldam, and T.J.H. Vlugt. "Polarizable Force Field for CO2 in M-MOF-74 Derived from Quantum Mechanics." In: *J. Phys. Chem. B* 122.42 (2018), pp. 24488–24498.

[118] T. Becker, A. Luba-Trigueo, J.M. Vicent-Luna, L.-C. Lin, D. Dubbeldam, S. Calero, and T.J.H. Vlugt. "Potential of Polarizable Force Fields for Predicting the Separation Performance of Small Hydrocarbons in M-MOF-74." In: *Phys. Chem. Chem. Phys.* 20 (2018), pp. 28848–28859.

[117] T.M. Becker, M. Wang, A. Kabra annd S.H. Jamali, M. Ramdin, D. Dubbeldam, C.A. Infante Ferreira, and T.J.H. Vlugt. "Absorption Refrigeration Cycles with Ammonia-Ionic Liquid Working Pairs Studied by Molecular Simulation." In: *Ind. Eng. Chem. Res.* 57.15 (2018), pp. 5442–5452.

[116] N.C. Burtch, J. Heinen, T.D. Bennett, D. Dubbeldam, and M.D. Allendorf. "Mechanical Properties in Metal-Organic Frameworks: Emerging Opportunities and Challenges for Device Functionality and Technological Applications." In: *Adv. Mater.* 30.37 (2018), p. 1704124.

[115] D. Dubbeldam, S. Calero, and T.J.H Vlugt. "iRASPA: GPU-Accelerated Visualization Software for Materials Scientists." In: *Mol. Simulat.* 44.8 (2018), pp. 653–676.

[114] J. Heinen and D. Dubbeldam. "On flexible force fields for metal-organic frameworks: recent developments and future prospects." In: *WIREs Comput. Mol. Sci.* 8.4 (2018), e1363.

[113] J. Heinen, A.D. Ready, T.D. Bennett, D. Dubbeldam, R.W. Friddle, and N.C. Burtch. "Elucidating the Variable-Temperature Mechanical Properties of a Negative Thermal Expansion Metal-Organic Framework." In: *ACS Appl. Mater. Interfaces* 10.25 (2018), pp. 21079–21083.

[112] I. Matito-Martos, A. Rahbari, A. Martin-Calvo, D. Dubbeldam, T.J.H. Vlugt, and S. Calero. "Adsorption equilbrium of nitrogen dioxide in porous materials." In: *Phys. Chem. Chem. Phys.* 20 (2018), pp. 4189–4199.

[111] J. Perez-Carbajo, D. Dubbeldam, S. Calero, and P. Merkling. “Diffusion Patterns in Zeolite MFI: the Cation Effect.” In: *J. Phys. Chem. C* 122.51 (2018), pp. 29274–29284.

[110] A. Rahbari, R. Hens, I.K. Nikolaidis, A. Poursaeidesfahani, M. Ramdin, I. G. Economou, O. A. Moultos, D. Dubbeldam, and T.J.H. Vlugt. “Computation of Partial Molar Properties Using Continuous Fractional Component Monte Carlo.” In: *Mol. Phys.* 116.21/22 (2018), pp. 331–3344.

[109] A. Rahbari, A. Poursaeidesfahani, A. Torres-Knoop, D. Dubbeldam, and T.J.H. Vlugt. “Chemical Potentials of Water, Methanol, Carbon Dioxide, and Hydrogen Sulfide at Low Temperatures using Continuous Fractional Component Gibbs Ensemble Monte Carlo.” In: *Mol. Simulat.* 44.5 (2018), pp. 405–414.

[108] Y. Tang, A. Kourtellaris, A.J. Tasiopoulos, S.J. Teat, D. Dubbeldam, G. Rothenberg, and S. Tanase. “Selective CO_2 adsorption in water-stable alkaline-earth based metal-organic frameworks.” In: *Inorg. Chem. Front.* 5.3 (2018), pp. 541–549.

[107] T.M. Becker, J. Heinen, D. Dubbeldam, L.-C. Lin, and T.J.H. Vlugt. “Polarizable Force Fields for CO2 and CH4 Adsorption in M-MOF-74.” In: *J. Phys. Chem. C* 121.8 (2017), pp. 4659–4673.

[106] J. Heinen, N.C. Burtch, K.S. Walton, and D. Dubbeldam. “Flexible Force Field Parameterization through Fitting on the Ab Initio derived Elastic Tensor.” In: *J. Chem. Theory. Comput.* 13.8 (2017), pp. 3722–3730.

[105] S.H. Jamali, M. Ramdin, T.M. Becker, A. Torres-Knoop, D. Dubbeldam, W. Buijs, and T.J.H. Vlugt. “Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations.” In: *Fluid Phase Equilbr.* 433 (2017), pp. 50–55.

[104] A. Luna-Triguero, J.M. Vicent-Luna, T.M. Becker, T.J.H. Vlugt, D. Dubbeldam, P. Gómez-Álvarez, and S. Calero. “Effective model for Olefin/Paraffin separation using (Co, Fe, Mn, Ni)-MOF-74.” In: *ChemistrySelect* 2.2 (2017), pp. 665–672.

[103] A. Poursaeidesfahani, M. de Lange, F. Khodadadian, D. Dubbeldam, M. Rigutto, N. Nair, and T.J.H. Vlugt. “Product Shape Selectivity of MFI, MEL, and BEA-type Zeolites in the Catalytic Hydroconversion of Heptane.” In: *J. Catal* 353 (2017), pp. 54–62.

[102] A. Poursaeidesfahani, R. Hens, A. Rahbari, M. Ramdin, D. Dubbeldam, and T.J.H. Vlugt. “Efficient application of Continuous Fractional Component Monte Carlo in the Reaction Ensemble.” In: *J. Chem. Theory. Comput.* 13.9 (2017), pp. 4452–4466.

[101] A. Poursaeidesfahani, R. Rahbari, A. Torres-Knoop, D. Dubbeldam, and T.J.H. Vlugt. “Computation of Thermodynamic Properties in the Continuous Fractional Component Monte Carlo Gibbs Ensemble.” In: *Mol. Simulat.* 43.3 (2017), pp. 189–195.

[100] A. Torres-Knoop, A. Poursaeidesfahani, D. Dubbeldam, and T.J.H. Vlugt. “Behavior of the Enthalpy of Adsorption in Nanoporous Materials close to Saturation Conditions.” In: *J. Chem. Theory. Comput.* 13.7 (2017), pp. 3326–3339.

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[3] H.E. Bal, R.A.F. Bhoedjang, R.F.H. Hofman, C.J.H. Jacobs, T. Kielmann, J. Maassen, R. van Nieuwpoort, J. Romein, L. Renambot, T. Rühl, R. Veldema, K. Verstoep, A. Baggio, G. Ballintijn, I. Kuz, G. Pierre, M.R. van Steen, A.S. Tanenbaum, G. Doornbos, D. Germans, H.J.W. Spoelder, E.-J. Baerends, S. van Gisbergen, H. Afsarmanesh, G.D. van Albada, A.S.Z. Belloum, D. Dubbeldam, Z.W. Hendrikse, L.O. Hertzberger, A.G. Hoekstra, K.A. Iskra, B.D. Kandhai, D.C. Koelma, F. van der Linden, B.J. Overeinder, P.M.A. Sloot, P.F. Spinnato, D.H.J. Epema, A. van Gemund, P.P. Jonker, A. Radulescu, C. van Reeuwijk, H.J. Sips, P.M.W. Knijnenburg, M. Lew, F. Sluiter, L. Wolters, H. Blom, and A.J. van der Steen. “The Distributed ASCI supercomputer project.” In: *Operating Systems Review* 34.4 (200), pp. 76–96.

3 Organization

Institutional responsibilities

2009 – present Design and management of local computing facilities of the Amsterdam Center for Multi-scale Modeling (ACMM) 0.2 fte [1]

2009 – present Lisa (national Dutch computer cluster, surfsara) advisory board

[1] Afspraak met het instituut: ”David Dubbeldam is in 2009 aangesteld als resultaat van de werving van een UD met profiel ”op gebied van computationele chemie en fysica met als bijzonder aandachts- terrein het ontwikkelen, implementeren en beheren van daaraan gerelateerde wetenschappelijke softwareapplicaties” en een ”verdeling van de tijdsbesteding aan enerzijds de onderwijs- en onderzoeksactiviteiten (inclusief het ontwikkelen en implementeren van numerieke methoden) en anderzijds de activiteiten op het gebied van beheer, ondersteuning van systeemsoftware en hardware zal ca. 80/20

2009-2010 Verhuiscoordinator Computational Chemistry (from Roetereiland to the Science Park Amsterdam).

Acting host at the UvA for John van Geuns and ACMM lectures

2019 Prof. Dr. Sofia Calero (University Pablo de Olavade, Seville, Spain), to be announced.

15 Oct. 2018 Dr. Nicholas C. Burtch (Sandia National Labs, USA), "Negative thermal expansion design strategies in metal-organic frameworks"

23 June 2017 Prof. Dr. Randall Snurr (Northwestern University, Evanston, USA), "Metal-Organic Frameworks as Tunable Platforms for Gas Storage, Chemical Separations, and Catalysis"

29 April 2016 Prof. Dr. Krista Walton (GTECH, Atlanta, USA), "Solving MOF instability: exploring factors that impact MOF degradation in the presence of water"

Organized seminars

18/19 Oct. 2017 "Molecular Simulation of Adsorption of Nanoporous Materials and Screening" (organizers: Sofia Calero, David Dubbeldam, and Thijs Vlugt), Seville, Spain.

3 Oct. 2016 "Molecular Simulation of Adsorption and Diffusion in Zeolites and Metal-Organic Frameworks" (organizers: David Dubbeldam, Thijs Vlugt and Sofia Calero), Seville, Spain.

19 Dec. 2016 "Molecular Simulation of Nanoporous Materials and Ionic Liquids" (organizers: David Dubbeldam, Thijs Vlugt and Sofia Calero), Delft, The Netherlands.

Organized schools

1-4 July 2019 School on Molecular simulations for adsorption and diffusion in nanoporous materials, and other applications (organizers: David Dubbeldam, Bogdan Kutcha, Thijs Vlugt, Sofia Calero, and Randall Snurr), Wroclaw, Poland.

7-18 Jan 2019 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

8-19 Jan 2018 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

30 May 2017 Tutorial on Molecular simulations for adsorption and diffusion in nanoporous materials, and other applications (organizers: Sofia Calero, David Dubbeldam, and Thijs Vlugt), DIFFER, Eindhoven.

9-20 Jan 2017 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

4-15 Jan 2016 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

5-16 Jan 2015 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

6-17 Jan 2014 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

7-18 Jan 2013 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

9-20 Jan 2012 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

3-14 Jan 2011 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

4-15 Jan 2010 Graduate winterschool on Understanding Molecular Simulation (organizers: Evert Jan Meijer, Bernd Ensing, and David Dubbeldam), Amsterdam.

Invited school lectures

29 June - 3 July 2020 School on Molecular simulations, and other applications (organizers: Bogdan Kutcha), Wroclaw, Poland.

Organized workshops

25-28 June 2018 Workshop on Molecular simulations for adsorption and diffusion in nanoporous materials, modeling of ionic liquids, and other applications (organizers: David Dubbeldam, Thijs Vlugt, Sofia Calero, and Randall Snurr), Delft, The Netherlands.

10-13 July 2018 Workshop on Molecular simulations for adsorption and diffusion in nanoporous materials, and other applications (organizers: David Dubbeldam, Randall Snurr, Thijs Vlugt, and Sofia Calero), Evanston, USA.

4 Teaching and supervision

Academic teaching certificates

Basiskwalificatie Onderwijs, 7 April 2014

Teaching activities

2018-2020 Development of an "Computer Aided Chemistry" track for chemistry master students, this new curriculum will include machine learning applied to chemistry. for chemistry master students.

2009 – present *Numerical Techniques*

Coordinator
Master's in Chemistry, track Molecular Simulation and Photonics
6 credits
During this course different numerical techniques, which can be used to solve sets of linear and nonlinear equations and differential equations, will be treated. With the aid of a computer several examples of relevant physical problems will be solved.

2009 – present *'Introduction Linux' and 'Learning C'*

Scientific Computing and Programming
6 credits, Coordinator: Luuk Vischer.
Master's in Chemistry and Physics, track ATOSIM
The course objective is to instill a broad understanding of how computers are utilized in scientific research, and impart practical skills in scientific programming and scripting.
This course is a collaborative effort involving the VU, UL, and UvA. It includes a total of six modules. Each student is expected to complete a minimum of four.

2017 – present First part of *'Introduction Scientific Programming for Chemists'*, BSc.

The course provides an introduction to programming concepts and tools used for scientific applications in chemistry.
Chemistry BSc., 6 credits, Coordinator: Luuk Vischer.

2009 – present *International Course 'MolSim' (Understanding Molecular Simulation tutorial)*

Organized by the Amsterdam Center for Multiscale Modelling
I wrote the exercises in 'C', and re-wrote and updated the exercises originally made by Thijs Vlugt for this course in Fortran-77. Acted as a lecturer and lab course assistant. Supervised two-week projects for UvA master-students.

Full promoter Phds

2017 – present Ilse Denekamp (University of Amsterdam, other promotor: Gadi Rothenberg).

2015 – 2020 Ahmadreza Rahbari, "Thermodynamics of Industrially Relevant Systems: Method Development and Applications", (Delft University), 8 first-author peer-reviewed articles. Thesis defense 16 April 2020.

2013 – 2018 Salvador R.G. Balestra (University Pablo de Olavide), 6 first-author peer-reviewed articles. Thesis defense 23 March 2018.

2009 – 2013 Juan-Jose Guiterrez-Sevillano (University Pablo de Olavide), thesis-defence July 2013, graduated Cum Laude, Extraordinary Prize for best thesis (current position: Postdoc Ghent University, Belgium).

Co-promoter Phds

2016 – present Sebastian Caro Ortiz (Delft University).

2014 – 2019 Tim Becker (Delft University), 6 first-author peer-reviewed articles, graduated 12 December 2019.

2014 – 2019 Ali Poursaidesfahani (Delft University), 8 first-author peer-reviewed articles, graduated 25 February 2019.

2014 – 2018 Jurn Heinen (University of Amsterdam, previously a master-student I supervised), graduated 16 October 2018.

2012 – 2016 Ariana Torres Knoop (University of Amsterdam), graduated Cum Laude 28 April 2016, 18 peer-reviewed articles (current position: Postdoc UvA).

2011 – 2015 Sayee Prasaad Balaji (Delft University), thesis-defence 23 Nov. 2015 (current position: Shell).

Highlight supervision master students

The project of master students R. Kools and F. Smit lead to a joined peer-reviewed paper: "Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions using CBMC, CFCMC, and CB/CFCMC", A. Torres-Knoop. N. Burtch, A. Poursaeidesfahani, S.P. Balaji, R. Kools, F. Smit, K.S. Walton, T.J.H. Vlugt, and D. Dubbeldam, J. Phys. Chem., 120(17), 9148-9159, 2016.

5 Scientific outreach

David Dubbeldam in the news

December 2019 Faculty and Institute Newsletter, Nature Chemistry article "Loading-dependent water effects on the structural properties of water stable MOFs", web link

Jan. 2019 Faculty/Institute Newsletter, "Successful International Winter School MolSim-2019", web-link.

28 Febr. 2018 iRASPA on SklogWiki, the open-edit encyclopedia dedicated to thermodynamics and statistical mechanics, web link

29 March 2018 Folia wetenschap: ”Chemicus maakt app om moleculen in 3D te analyseren” door Marleen Hoebe, Folia-link.

30 March 2018 Macs in Chemistry article ”iRASPA: GPU-accelerated visualization software for materials scientists”, Article-link

March 2018 ”Sophisticated free app for molecular visualization”, Van ’t Hoff Institure for Molecular Sciences, web link

28 March 2018 Emmerce, Industry Wire, ”Uitgebreide gratis app voor moleculaire visualisatie”, web-link

12 April 2018 ”Geavanceerde gratis app iRASPA voor moleculaire visualisatie”, web-link

19 April 2018 amsterdamsciencepark.nl: Novel, Water-stable Metal-Organic Framwork for Selective CO2 adsorption web-link.

May 2016 Faculty and Institute Newsletter ”Cum Laude PhD defence Ariana Torres Knoop”, web-link.

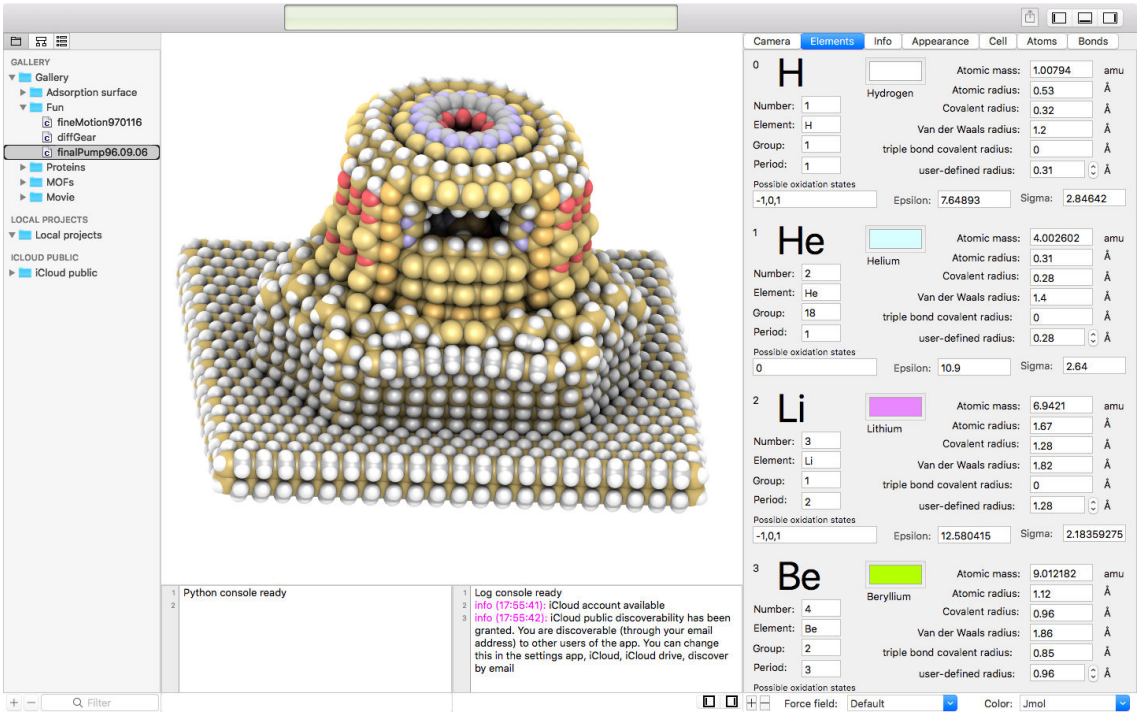
5 Sept. 2012 Onderzoek uitgelicht: chemicus David Dubbeldam, web-link.

6 Valorization

Valorization accomplishments

RASPA RASPA is a software package, developed by D. Dubbeldam, for simulating adsorption and diffusion of molecules in flexible nanoporous materials. The code implements the latest state-of-the-art algorithms for Molecular Dynamics and Monte Carlo in various ensembles including symplectic/measure-preserving integrators, Ewald summation, Configurational-Bias Monte Carlo, Continuous Fractional Component Monte Carlo, Reactive Monte Carlo, and Baker’s minimization. Applications of RASPA include computing coexistence properties, adsorption isotherms for single and multiple components, self- and collective diffusivities, reaction systems, and visualization. After 10 years of development, the software is now released under the GNU General Public License in 2016 (D. Dubbeldam, S. Calero, D.E. Ellis, R.Q. Snurr, *Mol. Simulat.* 2016). The package is now in use by over 30 research groups and institutions, including groups at the University of Amsterdam, Technical University of Delft, Georgia Tech (Atlanta, USA), Northwestern University (Evanston, USA), Shell (Amsterdam), and CSIRO (Melbourne, Australia).

iRASPA iRASPA is a visualization package (with editing capabilities) aimed at material science. Examples of materials are metals, metal-oxides, ceramics, biomaterials, zeolites, clays, and metal-organic frameworks. iRASPA is exclusively for macOS and as such can leverage the latest visualization technologies with stunning performance. iRASPA extensively utilizes GPU computing. For example, void-fractions and surface areas can be computed in a fraction of a second for small/medium structures and in a few seconds for very large unit cells. It can handle large structures (hundreds of thousands of atoms), including ambient occlusion, with high frame rates. The software is freely available from the Appstore, and described in a recently published paper (D. Dubbeldam, S. Calero, T.J.H. Vlugt, “iRASPA: GPU-Accelerated Visualization Software for Materials Scientists”, Mol. Simulat. 2018).



April 27, 2020