

Invited talks Veronique Van Speybroeck

2025

Invited talk

[Nanostructured materials for future technologies](#) , V. Van Speybroeck , Quetelet colleges , Ghent, Belgium ,
Tue, 25/11/2025

Invited talk

[Nanogestructureerde materialen als sleutel voor toekomstige technologieën](#) , V. Van Speybroeck ,
Wetenschappelijke nascholing , Ghent, Belgium , **Tue, 04/11/2025**

Invited talk

[Pushing the boundaries of simulations to model nanoporous materials for emerging technologies: How to bridge length and time scales while keeping quantum accuracy?](#) , V. Van Speybroeck , Online seminar at
Microsoft Quantum , online , **Thu, 30/10/2025**

Invited talk

[Pushing the limits of computational chemistry: the phase diagram of water](#) , M. Bocus, T. Braeckvelt, P.
Dobbelaere, A. Maet, W. Temmerman, S. Vandenhoute, S. Vanlommel, J. Vekeman, V. Van Speybroeck ,
EuroHPC User Days 2025 , Copenhagen, Denmark , **Tue, 30/09/2025 to Wed, 01/10/2025**

Keynote

[New frontiers in modeling adsorption in metal-organic frameworks accounting for flexibility and accurate intermolecular interactions](#) , V. Van Speybroeck, R. Goeminne, S. Ravichandran, T. Verstraelen, L. Vanduyfhuys
, 6th European Conference on Metal Organic Frameworks and Porous Polymers , Heraklion, Crete-Greece ,
Sun, 21/09/2025 to Wed, 24/09/2025

Invited talk

[New frontiers in modeling nanoporous materials and their applications at the crossroads of quantum mechanics, statistical physics and machine learning](#) , V. Van Speybroeck , Van Marum Colloquium , Leiden, The
Netherlands , **Thu, 04/09/2025**

Invited talk

[Operando modeling of nanoporous materials at the crossroads of quantum mechanics, statistical physics and machine learning](#) , V. Van Speybroeck , Psi-k conference , EPFL, Lausanne , **Mon, 25/08/2025 to Thu,
28/08/2025**

Plenary

[New avenues in modelling realistic nanoporous materials at operating conditions](#) , V. Van Speybroeck , 13th
Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC) , Oslo,
Norway , **Sun, 22/06/2025 to Fri, 27/06/2025**

Keynote

[Bridging Length and Time Scales in Catalysis for C1 Chemistry: From the Molecule to the Catalyst Particle Level](#)
, V. Van Speybroeck , 29th North American Meeting of the North American Catalysis Society (NAM29) , Atlanta,
GA, USA , **Sun, 08/06/2025 to Fri, 13/06/2025**

Invited talk

[New avenues in modeling nanoporous materials and their applications at crossroads of quantum mechanics, statistical physics and machine learning](#) , V. Van Speybroeck , Solvay Colloquia , Brussels, Belgium , **Mon,
12/05/2025**

Invited talk

[New avenues in modelling zeolite catalysis at operating conditions bridging length and time scales](#) , V. Van
Speybroeck , ITQ Severo Ochoa Lecture , Valencia, Spain , **Thu, 08/05/2025**

Invited talk

[Nanogestructureerde materialen als sleutel voor toekomstige technologieën](#) , V. Van Speybroeck ,

Minisymposium: "Het verleden ontcijferen, de toekomst zien", Algemene vergadering, Koninklijke Vlaamse Academie van België voor wetenschappen en kunsten , Brussels, Belgium , **Tue, 22/04/2025**

Plenary

[Multiscale Approaches from Molecular Design to Industrial Application: The Role of Machine Learning in Optimizing Catalytic Processes](#) , V. Van Speybroeck , Catalysis Connected , Rotterdam, The Netherlands , **Wed, 16/04/2025 to Thu, 17/04/2025**

Invited talk

[Nanostructured materials for future technologies](#) , V. Van Speybroeck , Quetelet colleges , Ghent, Belgium , **Tue, 01/04/2025**

Invited talk

[Machine Learning potentials for modeling realistic nanostructured materials and their applications](#) , V. Van Speybroeck , Meeting on Psiflow ML Potentials for Perovskites , Eindhoven, The Netherlands , **Mon, 27/01/2025**

Invited talk

[A dynamics view on zeolite catalysis at operating conditions bridging length and time scales](#) , V. Van Speybroeck , The 11th UK Catalysis Conference , Loughborough, United Kingdom , **Wed, 08/01/2025 to Fri, 10/01/2025**

2024

Invited talk

[New avenues in modeling nanoporous materials and their applications at crossroads of quantum mechanics, statistical physics and machine learning](#) , V. Van Speybroeck , Seminar at iit Atomistic Simulations , Genova, Italy , **Thu, 21/11/2024**

Invited talk

[Challenges and opportunities in modeling functional nanostructured materials for future technologies](#) , V. Van Speybroeck , ISCC Day , Utrecht, The Netherlands , **Fri, 15/11/2024**

Invited talk

[Modeling functional nanostructured materials for future technologies at the intersection of quantum mechanics, statistical physics and machine learning](#) , V. Van Speybroeck , Vereniging voor Natuurkundigen (VVN), Ghent University , Ghent, Belgium , **Thu, 07/11/2024**

Invited talk

[Machine learning potentials to bridge the gap between theory and experiments in zeolite catalysis](#) , M. Bocus, S. Vandenhoute, V. Van Speybroeck , Nanoinnovation 2024 , Rome, Italy , **Mon, 09/09/2024 to Fri, 13/09/2024**

Invited talk

[Machine Learning Potentials for nanostructured materials and their applications](#) , V. Van Speybroeck , Workshop: A TimeWarp in Digital Chemical Discoveries , Leiden, Netherlands , **Mon, 02/09/2024 to Fri, 06/09/2024**

Keynote

[A dynamics view on zeolite catalysis at operating conditions bridging length and time scales](#) , V. Van Speybroeck , 18th International Congress on Catalysis (ICC18) , Lyon, France , **Sun, 14/07/2024 to Fri, 19/07/2024**

Plenary

[Operando modelling of functional nanostructured materials for future technologies](#) , V. Van Speybroeck , Doctoral Workshop - PhD in Chemistry - Universitat Autònoma de Barcelona (UAB) , Barcelona, Spain , **Mon, 10/06/2024**

Invited talk

[New Frontiers in Modeling Complex Catalytic Cycles at Operating Conditions Bridging Length and Time Scales](#) , V. Van Speybroeck , ICIQ Seminar Programme , Tarragona (Spain) , **Fri, 19/04/2024**

Invited talk

[From quantum mechanics to machine learning : Bridging length and time scales in modeling nanoporous materials at operating conditions](#) , V. Van Speybroeck , Seminar Trinity College Dublin , Dublin, Ireland , **Fri, 15/03/2024**

2023

Honorary lectureship

[New Frontiers in Modeling Nanoporous Materials for Catalysis, Diffusion and Adsorption](#) , V. Van Speybroeck , The Dr. Karl Wamslser Innovation Award Symposium 2023 – Advancing Catalysis Science , Garching bei München (Germany) , **Thu, 09/11/2023**

Invited talk

[Challenges in modelling realistic metal-organic frameworks at operating conditions](#) , V. Van Speybroeck , Nobel Symposium NS193: Metal-organic frameworks – Fundamental science enabling transformative materials , Karlskoga, Sweden , **Tue, 19/09/2023 to Fri, 22/09/2023**

Invited talk

[Operando modelling of functional nanostructured materials for future technologies](#) , V. Van Speybroeck , One-day symposium - sorption, transport and catalysis in metal-organic frameworks , Uppsala, Sweden , **Mon, 18/09/2023**

Invited talk

[Resolving Complex Catalytic Cycles with Modeling Techniques Bridging Length and Time Scales](#) , V. Van Speybroeck , Gordon Research Conference - Expanding the Horizons of Porous Materials Design and Applications , Andover, United States , **Sun, 06/08/2023 to Fri, 11/08/2023**

Invited talk

[On the challenges of simulating accurate adsorption properties and their data management](#) , V. Van Speybroeck, L. Vanduyfhuys , "Digital Adsorption Data Space" - A IUPAC Task Force Symposium , Online , **Tue, 30/05/2023**

Honorary lectureship

[Hassel lecture 2023 - From quantum mechanics to machine learning: Bridging length and time scales in modeling nanoporous materials at operating conditions](#) , V. Van Speybroeck , University of Oslo , Oslo (Norway) , **Fri, 26/05/2023**

Honorary lectureship

[Hassel lecture 2023 - Operando modelling functional nanostructured materials for sustainable chemistry, nanosensing and clean energy](#) , V. Van Speybroeck , University of Oslo , Oslo (Norway) , **Thu, 25/05/2023**

Invited talk

[Resolving complex catalytic cycles with modeling techniques bridging length and time scales](#) , V. Van Speybroeck , Solvay Workshop "New ways to do chemistry Emerging technologies for synthetic methodology" , Brussels (Belgium) , **Mon, 24/04/2023 to Wed, 26/04/2023**

Invited talk

[Challenges in modeling spatiotemporal phenomena in metal-organic frameworks](#) , V. Van Speybroeck , Dynamic Materials , Crystals and Phenomena Conference (DynaMIC23) , Fribourg (Switzerland) , **Wed, 22/03/2023 to Fri, 24/03/2023**

Invited talk

[Operando modeling of realistic functional nanoporous materials for sustainable chemistry, nanosensing and clean energy](#) , V. Van Speybroeck , Colloquium at l'école nationale supérieure de chimie de Paris - PSL , Paris (France) , **Wed, 08/02/2023**

2022

Keynote

[Modeling Dynamic Processes in Realistic Nanostructured Materials at Operating Conditions.](#) , V. Van Speybroeck , Annual Meeting of the Quantum and Computational Chemistry Chapter of the Norwegian Chemical Society (NKS) , Bergen, Norway , **Mon, 28/11/2022 to Tue, 29/11/2022**

Invited talk

[Towards modeling spatiotemporal processes in metal-organic frameworks](#) , V. Van Speybroeck, S. Vandenhoute , MOF2022 , Dresden, Germany , **Sun, 04/09/2022 to Wed, 07/09/2022**

Invited talk

[Modelling realistic nanoporous materials at operating conditions](#) , V. Van Speybroeck , 5th Annual UK Porous Materials Conference , University of Strathclyde, Glasgow , **Mon, 13/06/2022 to Tue, 14/06/2022**

Invited talk

[Modelling realistic nanoporous materials at operating conditions](#) , V. Van Speybroeck , Supercomputer modelling of advanced materials , London, United Kingdom , **Mon, 06/06/2022 to Tue, 07/06/2022**

Invited talk

[A molecular modeling perspective on the C1 chemistry for light olefin and aromatics formation over zeolites](#) , V. Van Speybroeck , Nordco2 consortium , Online , **Thu, 02/06/2022**

Invited talk

[Computationally understanding and designing functional materials for energy applications: From nanoscale to realistic mesoscale models](#) , S.M.J. Rogge, V. Van Speybroeck , CChESMate 1st Meeting: Climate Change and Energy Solutions through Materials Science , Lille, France , **Thu, 28/04/2022 to Fri, 29/04/2022**

Invited talk

[Round-table discussion on the impact of crystal size and morphology on framework materials](#) , V. Van Speybroeck, R. Schmid, S. Kitagawa, D. Fairen-Jimenez, S. Wuttke , Online Symposium The Influence of Crystal Size & Morphology on Framework Materials , Online , **Thu, 10/02/2022**

2021

Invited talk

[Operando modeling of realistic functional nanoporous materials](#) , V. Van Speybroeck , IMX Seminar - Fall Series , Lausanne, Switzerland , **Mon, 27/09/2021 to Mon, 13/12/2021**

Invited talk

[Operando modeling of realistic functional nanoporous materials](#) , V. Van Speybroeck , ISIS Conference , Strasbourg, France , **Mon, 13/09/2021**

Invited talk

[Towards modeling spatiotemporal processes within nanoporous materials](#) , V. Van Speybroeck , Federation of European Zeolite Associations Conference (FEZA 2021) , virtual , **Mon, 05/07/2021 to Fri, 09/07/2021**

Invited talk

[Operando modeling of zeolite catalyzed processes using first principle molecular dynamics approaches](#) , V. Van Speybroeck , International Conference on Theoretical Aspects of Catalysis , Online Scientific Meeting , **Mon, 14/06/2021 to Wed, 30/06/2021**

Invited talk

[How the nature, transport and reactivity of confined hydrocarbons affects the lifetime and selectivity of methanol conversion catalysts](#) , V. Van Speybroeck , ACS Spring 2021 , Live Speaker Presentation , **Mon, 05/04/2021 to Fri, 30/04/2021**

2020

Invited talk

[Atomistic insight in the flexibility and heat transport properties of the stimuli-responsive metal-organic](#)

[framework MIL-53\(Al\) for water-adsorption applications using molecular simulations](#) , V. Van Speybroeck , Cooperative phenomena in framework materials: Faraday Discussion , UK (online) , **Tue, 13/10/2020 to Fri, 16/10/2020**

2019

Invited talk

[Unraveling the Thermodynamic Criteria for Size-Dependent Spontaneous Phase Separation in Soft Porous Crystals](#) , S.M.J. Rogge, M. Waroquier, V. Van Speybroeck , FlexMOF Symposium 2019 , Dresden, Germany , **Tue, 03/12/2019 to Thu, 05/12/2019**

Invited talk

[Molecular modeling at the Center for Molecular Modeling](#) , V. Van Speybroeck , DSM , The Netherlands , **Fri, 29/11/2019**

Invited talk

[Molecular modeling at operating conditions within zeolite catalysis](#) , V. Van Speybroeck , Nankai University , Tianjin, China , **Fri, 22/11/2019**

Invited talk

[Operando modelling of the dynamic behaviour of Metal Organic Frameworks](#) , V. Van Speybroeck , A Nature Conference: Physical Properties of Metal-Organic Frameworks , Tianjin, China , **Tue, 19/11/2019 to Thu, 21/11/2019**

Invited talk

[Molecular modeling at operating conditions within zeolite catalysis](#) , V. Van Speybroeck , State Key Laboratory of Coal Conversion (SKLCC) , Taiyuan, Shanxi, China , **Tue, 19/11/2019**

Invited talk

[Towards a molecular understanding of the flexible behavior of Metal-Organic Frameworks](#) , V. Van Speybroeck , Technical University Dresden , Dresden, Germany , **Tue, 12/11/2019**

Plenary

[A molecular-level perspective into the properties and dynamic behavior of metal-organic frameworks](#) , V. Van Speybroeck , EuroMOF2019 , Paris, France , **Sun, 27/10/2019 to Wed, 30/10/2019**

Invited talk

[Solvay conference in Chemistry : Operando modeling of functional nanoporous materials](#) , V. Van Speybroeck , 25th Solvay Conference on Chemistry - Computational Modeling: From Chemistry to Materials to Biology , Solvay, Brussels , **Wed, 16/10/2019 to Sat, 19/10/2019**

Invited talk

[Molecular modeling at operating conditions for zeolite catalyzed hydrocarbon conversions](#) , V. Van Speybroeck , 2019 IUPAC World Chemistry Congress , Paris, France , **Tue, 09/07/2019**

Plenary

[Unraveling the nature of reactive intermediates and prevailing pathways within zeolite catalysis by first principle molecular modeling](#) , V. Van Speybroeck , UK Catalysis Hub Spring Conference 2019 , Oxford, United Kingdom , **Thu, 02/05/2019 to Fri, 03/05/2019**

Honorary lectureship

[Unraveling complex chemical and physical transformations in nanoporous materials at operating conditions](#) , V. Van Speybroeck , Moscowitz Memorial Lectureship in Chemistry , Minneapolis, MN, USA , **Tue, 05/02/2019**

2018

Invited talk

[Molecular modeling within zeolite catalysis: Examples from the Methanol-to-Olefin process and olefin cracking](#) , V. Van Speybroeck , UOP , Des Plaines, IL, USA , **Wed, 07/11/2018**

Invited talk

[Modeling complex chemical and physical transformations in nanoporous materials at operating conditions](#) , V. Van Speybroeck , Northwestern University, Center for Catalysis and Surface Science , Evanston, Illinois, USA , **Mon, 05/11/2018**

Honorary lectureship

[Modeling nanoporous materials at the nanoscale](#) , V. Van Speybroeck , Eindhoven University of Technology , Eindhoven, The Netherlands , **Thu, 13/09/2018**

Honorary lectureship

[Modeling complex chemical and physical transformations in nanoporous materials at operating conditions](#) , V. Van Speybroeck , Eindhoven University of Technology , Eindhoven, The Netherlands , **Wed, 12/09/2018**

Honorary lectureship

[Modeling complex chemical and physical transformations in nanoporous materials at operating conditions](#) , V. Van Speybroeck , Twente University , Twente, The Netherlands , **Tue, 11/09/2018**

Honorary lectureship

[Modeling complex chemical and physical transformations in nanoporous materials at operating conditions](#) , V. Van Speybroeck , Utrecht University , Utrecht, The Netherlands , **Thu, 06/09/2018**

Honorary lectureship

[Modeling nanoporous materials at the nanoscale](#) , V. Van Speybroeck , Utrecht University , Utrecht, The Netherlands , **Wed, 05/09/2018**

Invited talk

[Towards modeling long-range disorder in MOFs: Development of a computational toolbox to extend the length scale in molecular simulations](#) , S.M.J. Rogge, R. Demuyne, A. De Vos, K. Hendrickx, K. Lejaeghere, G. Maurin, S. Vandenbrande, S. Vandenhoute, P. Van der Voort, L. Vanduyfhuys, T. Verstraelen, M. Waroquier, J. Wieme, V. Van Speybroeck , CECAM workshop: Multi-scale modelling of flexible and disordered porous materials , Paris, France , **Mon, 11/06/2018 to Wed, 13/06/2018**

Invited talk

[First principle MD simulations for complex chemical transformations in nanoporous materials](#) , V. Van Speybroeck , Symposium: Chemical Bonding in the 21st Century - A one day symposium in honor of Professor Roald Hoffmann , Brussels, Belgium , **Mon, 28/05/2018**

Plenary

[Molecular modeling within zeolite catalysis: The methanol-to-olefin process as a case study](#) , V. Van Speybroeck , 255th ACS National Meeting & Exposition , New Orleans, USA , **Sun, 18/03/2018 to Thu, 22/03/2018**

Plenary

[Molecular modeling within zeolite catalysis : The Methanol-to-Olefin process as a case study](#) , V. Van Speybroeck , NCCC XIX , Noordwijkerhout, The Netherlands , **Mon, 05/03/2018 to Wed, 07/03/2018**

2017

Keynote

[Towards a molecular level understanding of metal-organic frameworks](#) , V. Van Speybroeck , EUROMAT 2017 , Thessaloniki, Greece , **Sun, 17/09/2017 to Fri, 22/09/2017**

Keynote

[Molecular Modeling in Methanol to Olefins reaction](#) , V. Van Speybroeck , Europacat 2017 , Florence, Italy , **Sun, 27/08/2017 to Thu, 31/08/2017**

2016

Invited talk

[First principles simulations of complex catalytic transformations in nanoporous materials](#) , V. Van Speybroeck , UK Catalysis Hub Winter Conference , Harwell Campus, United Kingdom , **Tue, 06/12/2016 to Wed, 07/12/2016**

Invited talk

[First principle modeling of catalysis and materials at the nanoscale](#) , V. Van Speybroeck , Chemical Research in Flanders Symposium , Blankenberge , **Mon, 24/10/2016 to Wed, 26/10/2016**

Invited talk

[Density-functional theory and experiment: a match made in heaven or in hell?](#) , K. Lejaeghere, V. Van Speybroeck, L. Vanduyfhuys, T. Verstraelen, the Delta collaboration, S. Cottenier , EMN Meeting 2016 on Computation and Theory , Las Vegas, NV, USA , **Mon, 10/10/2016 to Fri, 14/10/2016**

Invited talk

[Orthogonal band gap engineering of UiO-66 frameworks through active control of defects](#) , K. Lejaeghere, A. De Vos, K. Hendrickx, S.M.J. Rogge, P. Van der Voort, V. Van Speybroeck , EMN Meeting 2016 on Active Matter , Las Vegas, NV, USA , **Mon, 10/10/2016 to Fri, 14/10/2016**

Invited talk

[First principle modeling of complex chemical transformations in zeolites and metal-organic frameworks](#) , V. Van Speybroeck , French Conference on Catalysis (FCCat1) , Frejus, France , **Mon, 23/05/2016 to Fri, 27/05/2016**

Invited talk

[Quality Control: Has Your DFT Code Been \$\Delta\$ -approved?](#) , K. Lejaeghere, V. Van Speybroeck, W. Poelmans, S. Cottenier , 2016 TMS Annual Meeting & Exhibition , Nashville, TN, USA , **Sun, 14/02/2016 to Thu, 18/02/2016**

2015

Invited talk

[First-Principle Modeling of Chemical and Physical Transformations in Complex Molecular Environments](#) , V. Van Speybroeck , 3rd meeting on Challenges in Computational Homogeneous Catalysis , Stockholm, Sweden , **Thu, 03/09/2015 to Fri, 04/09/2015**

Keynote

[Understanding The Flexibility In Metal-Organic Frameworks From molecular To Thermodynamic Insights](#) , L. Vanduyfhuys, S. Vandenbrande, R. Demuynck, S.M.J. Rogge, A. Ghysels, T. Verstraelen, M. Waroquier, V. Van Speybroeck , CHITEL2015 , Torino, Italy , **Sun, 26/07/2015 to Fri, 31/07/2015**

Invited talk

[Carbon Capture Turned Upside Down: High-Temperature Adsorption & Low-Temperature Desorption \(HALD\)](#) , L. Joos, K. Lejaeghere, J. Huck, V. Van Speybroeck, B. Smit , Visit group of Prof. Geoffroy Hautier , Louvain-la-Neuve , **Tue, 23/06/2015**

Invited talk

[Can catalysts be designed using theory?](#) , V. Van Speybroeck , Satellite Meeting "Catalysis making the world a better place" , Chicheley Hall, Buckinghamshire , **Wed, 10/06/2015 to Thu, 11/06/2015**

Invited talk

[DFT and experiment: a match made in heaven or in hell?](#) , K. Lejaeghere, L. Vanduyfhuys, V. Van Speybroeck, S. Cottenier , Abidev2015 , Liège, Belgium , **Tue, 28/04/2015 to Thu, 30/04/2015**

Invited talk

[Exploring new frontiers in modeling complex chemical transformations in nanoporous materials](#) , V. Van Speybroeck , UC Berkeley , Berkeley, USA , **Thu, 26/02/2015**

Invited talk

[Exploring new frontiers in modeling complex chemical transformations in nanoporous materials](#) , V. Van

Speybroeck , Machine Learning for Many-Particle Systems , Los Angeles, CA, USA , **Mon, 23/02/2015 to Fri, 27/02/2015**

2014

Invited talk

[Towards simulations of complex chemical conversions in zeolites](#) , V. Van Speybroeck, K. De Wispelaere , Dutch Zeolite Association “On Hybrids and Zeolites” , Gent , **Tue, 07/10/2014**

Invited talk

[Critical analysis of liquid structure models](#) , M. Van Houteghem, A. Ghysels, T. Verstraelen, W. Poelmans, M. Waroquier, V. Van Speybroeck , WATOC 2014 , Santiago de Chile, Chile , **Sun, 05/10/2014 to Fri, 10/10/2014**

Invited talk

[Three years of computer experiments about Po and LBE: what did we learn?](#) , K. Rijpstra, A. Van Yperen-De Deyne, V. Van Speybroeck, S. Cottenier , SEARCH/MAXIMA 2014 International Workshop , Karlsruhe, Germany , **Fri, 03/10/2014**

Invited talk

[Het belang van moleculaire modellering bij het ontwerp van chemische processen en nanoporeuze materialen](#) , V. Van Speybroeck , Lezing binnen de klasse Natuurwetenschappen van de KVAB ter gelegenheid van inauguratie als nieuw lid van de academie , België , **Sun, 07/09/2014**

Invited talk

[Ab initio modeling for the design of TCO's: structural properties](#) , K. Rijpstra, K. Lejaeghere, M. Waroquier, V. Van Speybroeck, S. Cottenier , The future of transparent conducting oxides , Hasselt, Belgium , **Tue, 26/08/2014**

Invited talk

[Model guided design of nanomaterials for catalysis and adsorption](#) , V. Van Speybroeck , 5th International conference on advanced nanomaterials , Aveiro, Portugal , **Wed, 02/07/2014 to Fri, 04/07/2014**

Invited talk

[Polonium in Accelerator Driven Systems: computer experiments meet lab experiments](#) , K. Rijpstra, A. Van Yperen-De Deyne, M. Waroquier, V. Van Speybroeck, S. Cottenier , PSI-seminar , Villigen (Switzerland) , **Fri, 09/05/2014**

Invited talk

[Towards applications of Metal-organic Frameworks through model-guided design](#) , V. Van Speybroeck , , Ruhr-Universität Bochum, Germany , **Fri, 21/02/2014**

Invited talk

[The Delta parameter: which precision has a meaning on physical results?](#) , S. Cottenier, K. Lejaeghere, V. Van Speybroeck , (presenting author: S. Cottenier), Pseudopotentials and PAW atomic data: beyond a "black art"? , Paris, France , **Tue, 28/01/2014 to Wed, 29/01/2014**

Invited talk

[How to validate pseudopotentials? Methods of comparison](#) , K. Lejaeghere, S. Cottenier, V. Van Speybroeck , (presenting author: K. Lejaeghere), CFCAM workshop 'Pseudopotentials and PAW atomic data: beyond a "black art"?' , Paris, France , **Tue, 28/01/2014 to Wed, 29/01/2014**

Invited talk

[The value of HPC for Molecular Modeling applications](#) , V. Van Speybroeck , VSC Users Day , Brussels, Internationaal Auditorium , **Thu, 16/01/2014**

Invited talk

[DFT vs. reality: the error budget](#) , S. Cottenier, K. Lejaeghere, J. Jaeken, V. Van Speybroeck , International workshop on computational physics and materials science ("Total energy and force methods") , Lausanne, Switzerland , **Thu, 09/01/2014 to Sat, 11/01/2014**

2013

Invited talk

[ACKS2: Atom-Condensed Kohn-Sham nd DFT approximated to 2nd order](#) , T. Verstraelen, P.W. Ayers, V. Van Speybroeck, M. Waroquier , Visit Guillaume Maurin , Montpellier, France , **Tue, 01/10/2013 to Sun, 03/11/2013**

Invited talk

[Extended Hirshfeld: robust charges & accurate ESPs](#) , T. Verstraelen, P.W. Ayers, V. Van Speybroeck, M. Waroquier , Visit Guillaume Maurin , Montpellier, France , **Tue, 01/10/2013 to Thu, 03/10/2013**

Invited talk

[First principle chemical kinetics of reactions in gas phase, solution and nanoporous materials](#) , V. Van Speybroeck , School on Atomistic Simulation Techniques , University of Antwerp , **Mon, 23/09/2013 to Tue, 24/09/2013**

Invited talk

[The ground state elemental crystals as a guideline for the assessment of solid state DFT accuracy](#) , K. Lejaeghere, V. Van Speybroeck, G. Van Oost, S. Cottenier , (presenting author K. Lejaeghere), NIST Workshop on Atomistic Simulations for Industrial Needs , Gaithersburg, MD, USA , **Tue, 13/08/2013 to Wed, 14/08/2013**

Invited talk

[The Mechanism of Methanol Conversion: Insight from Extended Cluster Models and Molecular Dynamics](#) , K. De Wispelaere, K. Hemelsoet, S.L. Moors, J. Van der Mynsbrugge, M. Waroquier, V. Van Speybroeck , 4th Annual Global Congress of Catalysis (GCC-2013) , Dalian, China , **Sat, 29/06/2013 to Mon, 01/07/2013**

Invited talk

[Inverse Materials Design for Tungsten Alloys](#) , K. Lejaeghere, S. Cottenier, V. Van Speybroeck , (presenting author S. Cottenier) International Workshop on High-throughput Materials Development , Ghent, Belgium , **Tue, 11/06/2013 to Wed, 12/06/2013**

Invited talk

[ACKS2: Atom-Condensed Kohn-Sham nd DFT approximated to 2nd order](#) , T. Verstraelen, P.W. Ayers, V. Van Speybroeck, M. Waroquier , Visit Konstantin Smirnov , Lille, France , **Fri, 18/01/2013**

2012

Invited talk

[Finding candidate materials for the first wall of fusion reactors by an inverse strategy](#) , K. Lejaeghere, S. Cottenier, M. Waroquier, V. Van Speybroeck , (presenting author S. Cottenier) MRS Fall Meeting , Boston, USA , **Sun, 25/11/2012 to Fri, 30/11/2012**

Invited talk

[ACKS2: Atom-Condensed Kohn-Sham nd DFT approximated to 2nd order](#) , T. Verstraelen, P.W. Ayers, V. Van Speybroeck, M. Waroquier , Visit Martin Müser , Jülich, Germany , **Mon, 29/10/2012 to Tue, 30/10/2012**

Invited talk

[Error bars for solid-state density-functional theory predictions](#) , K. Lejaeghere, G. Van Oost, V. Van Speybroeck, S. Cottenier , (presenting author S. Cottenier), 17th ETSF Workshop on Electronic Excitations , Coimbra, Portugal , **Mon, 01/10/2012 to Fri, 05/10/2012**

Invited talk

[Model-guided design of Metal-organic Frameworks](#) , V. Van Speybroeck , Universiteit van Amsterdam , Amsterdam , **Wed, 26/09/2012**

Invited talk

[Model-guided design of Metal-Organic Framework](#) , V. Van Speybroeck , Invited seminar at van 't Hoff Institute for Molecular Sciences - University of Amsterdam , Amsterdam , **Wed, 26/09/2012**

Invited talk

[The ground state elemental crystals as a guideline for the assessment of solid state DFT accuracy](#) , K.

Lejaeghere, V. Van Speybroeck, G. Van Oost, S. Cottenier , (presenting author K. Lejaeghere), CECAM Workshop on Validation and Verification in Electronic-Structure calculations: state of the art and perspectives , Lausanne, Switzerland , **Wed, 05/09/2012 to Fri, 07/09/2012**

Invited talk

[Error bars on DFT predictions: sense or nonsense?](#) , K. Lejaeghere, G. Van Oost, V. Van Speybroeck, S. Cottenier

, (presenting author S. Cottenier), 19th WIEN2k Workshop , Waseda University, Tokyo, Japan , **Mon, 03/09/2012 to Fri, 07/09/2012**

Invited talk

[First principle chemical kinetics in zeolites: The MTO process as a case study](#) , V. Van Speybroeck , Technische

Universität Munchen (J. Lercher group) , München, Germany , **Tue, 10/01/2012**

2011

Invited talk

[Computational materials design for electricity generation in the 22nd century](#) , S. Cottenier, K. Lejaeghere, V.

Van Speybroeck , (presenting author S. Cottenier) 4th Workshop on novel methods for electronic structure calculations, and 1st southamerican congress on materials , La Plata (Argentina) , **Wed, 02/11/2011 to Fri, 04/11/2011**

Invited talk

[First principle kinetic studies of zeolite catalyzed reactions](#) , V. Van Speybroeck , Department of Chemistry,

University of Oslo , Oslo, Norway , **Mon, 14/02/2011 to Wed, 16/02/2011**

2010

Invited talk

[Materials modeling at the nanoscale](#) , V. Van Speybroeck , Umicore , Olen, Belgium , **Tue, 02/11/2010**

Invited talk

[First principle modeling of conjugated polymer formation](#) , V. Van Speybroeck , , Boğaziçi University, Bebek,

Istanbul, Turkey , **Wed, 22/09/2010**

2008

Invited talk

[The methanol to olefin process from theoretical perspective](#) , V. Van Speybroeck , ESEP European Symposium

2008, Advanced Materials , Exxon Mobil, Belgium , **Wed, 17/12/2008**

Invited talk

[First principle chemical kinetics : From gas phase to supramolecular systems](#) , V. Van Speybroeck ,

WATOC2008 , Sydney, Australia , **Sun, 14/09/2008 to Fri, 19/09/2008**

Invited talk

[Research activities CMM](#) , V. Van Speybroeck , , Jülich Forschungszentrum, Jülich, Germany , **Fri, 29/08/2008**

Invited talk

[On the structures and Reactivity of Cationic Rhodium Monodendate Phosphoramidites for hydrogenation of](#)

[olefins](#) , V. Van Speybroeck , , DSM, Geleen, The Netherlands , **Tue, 05/08/2008**

Invited talk

[First principle chemical kinetics: From isolated molecules to supramolecular systems](#) , V. Van Speybroeck ,

Eurokin's 10th Anniversary meeting , Lyon, France , **Mon, 19/05/2008 to Tue, 20/05/2008**

Invited talk

[Ab initio reaction kinetics : Use of internal hindered rotors](#) , V. Van Speybroeck , Combustion Chemistry Centre, National University of Galway , Galway, Ireland , **Mon, 11/02/2008 to Tue, 12/02/2008**

2007

Invited talk

[Simulating reactions in organic solvents](#) , V. Van Speybroeck , Invited stay in the group of Prof. Aviyente , Bogazici University, Bebek, Istanbul, Turkey , **Thu, 26/04/2007**

2006

Invited talk

[Reactivity of Cationic Rhodium/MonoPhos Lewis-acid catalysts for hydrogenation of olefins](#) , V. Van Speybroeck , Workshop , Center for Surface Chemistry and Catalysis, Leuven , **Thu, 07/12/2006 to Fri, 08/12/2006**

Invited talk

[On the activity of rhodium phosphoramidite asymmetric hydrogenation catalysts](#) , V. Van Speybroeck , , DSM, Geleen, The Netherlands , **Tue, 17/10/2006**

2005

Invited talk

[Identification of radiation-induced radicals in crystalline sugars: comparing ab-initio calculations with magnetic resonance experiments](#) , E. Pauwels, V. Van Speybroeck, M. Waroquier , , Invited stay in the group of Prof. G. Grampp, ESR and Photochemistry group, Technische Universität Graz, Austria , **Tue, 13/12/2005 to Wed, 14/12/2005**

Invited talk

[Chemical kinetics of organic and organometallic reactions through molecular modeling](#) , V. Van Speybroeck , , Invited stay in the group of Prof. Aviyente, Istanbul, Turkey , **Tue, 22/11/2005 to Fri, 25/11/2005**

2002

Invited talk

[Kinetics of 1-hexene isomerization with methane sulphonic acid from first principles](#) , V. Van Speybroeck, D. Van Neck, M. Waroquier , Eurokin meeting , Terneuzen, The Netherlands , **Mon, 25/11/2002**

2001

Invited talk

[Thermal degradable polycarbonates](#) , V. Van Speybroeck , , Agfa Gevaert, Belgium , **Thu, 29/11/2001**

Invited talk

[Kinetic parameters of chemical reactions calculated from first principles](#) , V. Van Speybroeck , EUROKIN (a European cooperation initiative on kinetics research) meeting , Louvain-la-Neuve , **Sun, 18/02/2001 to Mon, 19/02/2001**