

**Alexander V. Neimark**

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Google Scholar Website: <http://scholar.google.com/citations?user=qI3rDSQAAAAJ&hl=en>

**A. PROFESSIONAL PREPARATION**

M.S.	1973	Mechanical Engineering, Lomonosov Moscow State University, Russia
Ph.D.	1977	Chemical Engineering, Institute of Chemical Industry, Moscow, Russia
D.Sc.	1988	Physical Chemistry, Lomonosov Moscow State University, Moscow, Russia

**B. APPOINTMENTS**

2006- Distinguished Professor, Chemical and Biochemical Engineering, Rutgers, New Brunswick, NJ  
2000-06 Research Director, Center for Modeling and Characterization of Nanoporous Materials, Textile Research Institute, Princeton, NJ  
1996-00 Principal Scientist, Textile Research Institute, Princeton, NJ  
1994-96 Professor Adjunct and Senior Research Associate, Dept. of Chemical Engineering, Yale University, New Haven, CT  
1989-94 Leading Scientist, Institute of Physical Chemistry, Moscow, Russia  
1977-88 Junior Scientist, Scientist, Senior Scientist, State R&D Institute of Chemical Industry, Moscow

**C. SELECTED PROFESSIONAL HONORS & APPOINTMENTS**

2022 Elected Director, International Adsorption Society  
2021 Visiting Professor, Chimie ParisTech, University of Science and Letters, Paris, France  
2019 Claude R. Hocott Lecture in Petroleum Engineering, University of Texas in Austin.  
2019 Thomas Young Centre Soiree Lecture. London, UK  
2019 Keynote Speaker. 13<sup>th</sup> International Conference of Fundamentals of Adsorption, Cairns, Australia  
2019 Fellow, International Adsorption Society  
2018 Distinguished Visiting Professor, Shinshu University, Nagano, Japan  
2018 Japan Science and Technology Agency CREST Award, Japan  
2018 Leverhulme Trust Visiting Professor, University College London, UK  
2018 Leverhulme Lecture Series in UK Universities: University College London, Cambridge University, University of Manchester, University of Bath, University of Edinburgh.  
2017 Keynote Speaker. 9<sup>th</sup> Sino-US Joint Conference of Chemical Engineering, Beijing, China  
2017 Invited Lecturer. VII International Conference "Diffusion Fundamental", Moscow, Russia  
2017 Invited Speaker. 6<sup>th</sup> Biot Conference on Poromechanics, 9-13 Jul 2017, Paris, France  
2016 Invited Lecturer. 12<sup>th</sup> Int. Conference on Fundamentals of Adsorption, Friedrichshafen, Germany  
2016 Board of Governors Award for Excellence in Research, Rutgers, New Brunswick, NJ  
2015 Honorary plenary session, Area 02E, AIChE annual meeting, Salt Lake City, UT  
2015 Recognition plaque for seminal contributions, AIChE Separation Division  
2015 Invited Talk. International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii  
2015 Keynote Speaker. 8<sup>th</sup> Sino-US Joint Conference of Chemical Engineering, Shanghai, China  
2015 Mork Family Visiting Scholar, University of Southern California, Los Angeles, CA.  
2014 Inviter speaker. The 13<sup>th</sup> International Ceramics Congress, Montecatini Terme, Italy  
2014 Invited speaker, CECAM Workshop "Dissipative Particle Dynamics", Lausanne, Switzerland  
2014 Editor, Colloid and Interface Science Communications, Elsevier  
2013-14 Visiting Professor, ENSCP - Chimie ParisTech, Paris, France  
2013 Tomas Young Center Soiree Lecture, King's College, London, UK  
2013 Distinguished Visiting Fellow, Royal Academy of Engineering, UK  
2013 Rutgers Faculty Ambassador  
2012 Fellow, American Institute of Chemical Engineers  
2012 Visiting Professor, Ecole Normale Superior, Paris, France  
2012 Keynote speaker. Int. Symposium on Zeolites and Microporous Materials, Hiroshima, Japan  
2011 Plenary speaker, AIChE Annual Meeting, Minneapolis, MN  
2011 Visiting Professor, Nanjing University, China  
2010 Plenary speaker, 10<sup>th</sup> International Conference on Fundamentals of Adsorption, Hyogo, Japan  
2009-11 Blaise Pascal International Chair, ENS Foundation, Paris, France  
2009 Invited speaker, Fall Meeting of Materials Research Society, Boston, MA  
2009 Invited lecturer, International Conference "Diffusion Fundamentals III", Athens, Greece  
2008 Merit Award, Rutgers University, USA  
2008 Invited Lecturer. 6<sup>th</sup> Congress of Int. Soc. Theoretical Chemical Physics, Vancouver, Canada  
2008 Invited Lecturer. 7<sup>th</sup> International Symposium on Polyelectrolytes, Coimbra, Portugal  
2007-13 Elected Member, Board of Directors, International Adsorption Society.

- 2007 Invited speaker. International Conference “Thermodynamics 2007, Rueil-Malmaison, France
- 2007 Keynote speaker. International Carbon Conference, Seattle, WA.
- 2006-14 Member, IUPAC Task Groups Characterization of Porous Materials and Physisorption of Gases
- 2006 Distinguished Visiting Professor, American University, Cairo, Egypt
- 2006 Invited lecturer. International Conference "Transport in polymeric membranes", Pula, Italy
- 2005 Most Cited Scientist, ISI Essential Science Indicators
- 2005 Stanley Katz Annual Memorial Lecture, City College, CCNY, New York
- 2005 Plenary speaker. 7th Int. Symp. Characterization of Porous Solids, Aix en Provence, France
- 2005 Keynote lecturer. International Symposium on Nanoporous Materials IV, Niagara Falls, Canada
- 2004-5 Visiting Scholar, Princeton University, Princeton, NJ
- 2004 Guggenheim Fellow, John Simon Guggenheim Memorial Foundation
- 2004-5 Adjunct Professor, Dept. of Materials Science and Engineering, Drexel U., Philadelphia, PA
- 2004 FUMEC Distinguished Lectureship Award, Mexican Academy of Sciences, Mexico
- 2004 Plenary speaker. 8th International Conference on Fundamentals of Adsorption, Sedona, AR
- 2003 Invited lecturer. 3rd Pacific Basin Conference on Adsorption Science and Technology, Korea
- 2003 Keynote lecturer. NATO-ASI on "Nanoengineered Nanofibrous Materials", Antalya, Turkey
- 2003 Invited speaker. MRS Fall Meeting, Boston, MA
- 2002 Invited Plenary Lecturer. Meeting of Chem. Soc. Japan, Tokyo, Japan, March 28-29, 2002.
- 2002 Keynote speaker. 6th Int. Symposium on Characterization of Porous Solids, Alicante, Spain
- 2001 Plenary Lectureship Award, Nanoscale Science & Engineering Symposium, AIChE, Reno, NV
- 2001 Plenary speaker. 7th Int. Conference on Fundamentals of Adsorption, Nagasaki, Japan
- 2000 Johnson & Johnson Focused Giving Program Award
- 2000 Plenary speaker, Pacific Basin Conf. on Adsorption Science & Technology, Brisbane, Australia
- 2000 Keynote Lecture. 2nd Int. Symposium on Mesoporous Molecular Sieves, Quebec City, Canada
- 2000 Invited speaker. MRS Fall Meeting, Boston
- 1988 Plenary speaker, 3rd Int. Symp. on Surface heterogeneity in Adsorption and Catalysis, Poland
- 1994 Fellow, Mandelbrot Foundation for Fractals, New Haven, CT
- 1993-4 Visiting Director of Research, National Center of Scientific Research, Poitiers, France
- 1992-3 DFG Visiting Professor, Johannes Gutenberg University, Mainz, Germany
- 1991-2 Humboldt Research Fellow, Humboldt Foundation, Bonn

#### **D. SYNERGISTIC & EDUCATIONAL ACTIVITIES**

1. Founder and Director of the Center for Modeling and Characterization of Nanoporous Materials, TRI/Princeton, Princeton, NJ, 1996-2006.
2. Director of the core technology project “Interactions of fluids with porous materials” co-sponsored by a group of U.S. and European industrial companies, TRI/Princeton, Princeton, NJ, 2000-2006.
3. Director of the Chemical and Biochemical Engineering Graduate Program, Rutgers, 2007-2010.
4. Co-PI, GAANN educational program on "Pharmaceutical Engineering", Rutgers, 2009-2014.
5. Member, IUPAC Task Groups on "Characterization of porous materials" and "Physisorption of Gases", 2006-2015.
6. Founder and Chairman of the International Workshops on Characterizations of Porous Materials (CPM), USA, 1997, 2000, 2003, 2006, 2009, 2012, 2015, 2018, 2024.
7. Chairman of the International Workshop on Nanocapillarity, USA, 2001.
8. Co-Chairman of the International Workshops on Adsorption in Compliant Solids, France, 2011, 2013.
9. Co-Chairman of Diffusion Fundamentals International Conference, USA, 2011.
10. US Co-Chair of the 7<sup>th</sup> Fundamental of Adsorption International Conference, Germany, 2016.
11. Organizer, Chairman, and Co-Chairman of sessions on Molecular Modeling of Adsorption, Characterization of Nanoporous Materials, Molecular Modeling and Design of Nanostructured Adsorbents, Theory and Simulation of Adsorption at the annual meetings of AIChE, 1999-2019.
12. Member of International Advisory Committees. International Conferences & Symposia on Computational Modeling and Simulation (Italy, 2004), Fundamentals of Adsorption (Japan, 2001; USA, 2004; Italy 2007, Japan, 2010, USA, 2013, Germany 2016, Australia 2019, USA 2022), Adsorption Science and Technology (Australia, 2000, Korea, 2003, China, 2006, Singapore, 2009), Characterization of Porous Solids (Spain, 2002; France, 2005, UK 2008, Germany 2011, Spain 2014, France 2017), European Excellence Project “INPORE”, 2008-2011, and others.
13. Editor. Colloid and Interface Science Communications, Elsevier, 2014-2016.
14. Editorial Board. Adsorption Science and technology
15. Guest Editor. Advances in Colloid and Interface Science, Colloids and Surfaces, Microporous and Mesoporous Materials.

**E. PUBLICATIONS:** 1 monograph, 11 edited volumes, 290+ peer-reviewed papers, 38,400+ citations, [h-index=76](#), see list below.

**F. PRESENTATIONS:** 200+ (in 1988-2019) invited lectures, seminars, keynotes, and plenary talks in the major national and international scientific meetings and leading research institutions worldwide, see list below.

**G. GRANT AWARDS AS PRINCIPAL INVESTIGATOR, Rutgers University, 2006-2023**

1. Modeling and Adsorption Characterization of Porous Materials, PI, Microtrac Instruments, Award amount \$60,000, 11/01/2023 – 10/31/2024.
2. INTERN Supplement: Deformation of Poroelastic Nanoporous Materials of Hierarchical Structure upon Adsorption of Gas Mixtures: Theory, Molecular Modeling and Experiments, PI, NSF – CBET (2224191/1834339), Award Amount: \$55,000, 09.01.22 - 08.31.23
3. Development of Tailored Metal Organic Framework Designer Monte Carlo/Density Functional Theory Kernels for Gas Adsorption Characterization, PI, MSI STEM R&D Consortium, Award amount \$78,000.00, 05.26.2022 – 06.30.2024
4. Coarse-grained modeling of surfactant and amino acid adsorption on dental biofilms. PI, Colgate-PalmOlive, Award Amount: \$75,000; 08.01.22-07.31.23.
5. Multiscale Modeling of Coronavirus Virions in the Respiratory System, PI, NSF\_DMR (2138052), Award Amount \$499,765, 07.01.2022 – 06.30.2026.
6. Development of Computational Models to Explore Interactions of Coronavirus Virions with Lung Surfactant Films, PI, NJ ACTS Pilot Project Grant Program, Award Amount \$50,000, 09.15.21-09.14.22.
7. Collaborative Research: Interactions of Airborne Engineered Nanoparticles with Lung Surfactant Films, PI, NSF-CBET, (2040302), Award Amount \$359,999, 06.16.2021 – 09.30.2024.
8. INTERN Supplement: Deformation of Poroelastic Nanoporous Materials of Hierarchical Structure upon Adsorption of Gas Mixtures: Theory, Molecular Modeling and Experiments, PI, NSF – CBET (2131157/1834339), Award Amount: \$55,000, 06.03.21 - 08.31.22 (11.30.22)
9. Advanced Methods for Pore Structure Characterization and Adsorption in Geological Materials, PI, ExxonMobil Corporation, Award Amount: \$150,000+159,500=\$309,500, 02.01.21 - 01.30.24
10. INTERN Supplement: Deformation of Poroelastic Nanoporous Materials of Hierarchical Structure upon Adsorption of Gas Mixtures: Theory, Molecular Modeling and Experiments, PI, NSF – CBET (2032245/1834339), Award Amount: \$55,000, 09.01.20 - 08.31.21
11. Computational Modeling of Xanthan Gum Solutions, PI, Colgate-PalmOlive, Award Amount: \$157,500; 06.01.19-10.31.21.
12. INTERN Supplement: Theoretical Foundations of Interaction Nanoparticle Chromatography, PI, NSF – CBET/GOALI (1839245), Award Amount: \$50,000, 03.01.19 - 02.28.20
13. Collaborative Research: Deformation of Poroelastic Nanoporous Materials of Hierarchical Structure upon Adsorption of Gas Mixtures: Theory, Molecular Modeling and Experiments, PI, NSF – CBET (1834339), Award Amount: \$278,259; 09.01.18 - 08.31.21
14. INTERN Supplement: Theoretical Foundations of Interaction Nanoparticle Chromatography, PI, NSF – CBET/GOALI (1839245), Award Amount: \$50,000, 09.01.18 - 02.28.19
15. Molecular Design of Biomimetic Lipid Membranes and Liposomes, PI, Rutgers Bush Biomedical Award, Award Amount: \$40,000, 09.01.18 - 08.31.20
16. Travel Grant for International Workshop on Characterization of Porous Materials, NSF (1818797), Co-PI, Award Amount: \$12,000, 04/01/2018 - 03/31/2019
17. GOALI: Theoretical Foundations of Interaction Nanoparticle Chromatography, PI, NSF CBET (1510993), Award Amount: \$300,000; 09.01.2015 -08.30.2019
18. Mass Transport, Kinetics, and Catalytic Activities of Multicatalyst Polyelectrolyte Membranes, PI, DTRA (HDTRA1-14-1-0015), Award Amount: \$1,569,777; 02.06.2014 - 07.14.2019
19. Characterization of Porous Materials, PI, Anton Paar QuantaTec Inc/ Quantachrome Instruments Award Amount: \$44,000/year, 05.01.07 - 12.31.19
20. Adhesion and Translocation of Nanoparticles through Lipid Membranes, PI, NSF CBET (1264702), Award Amount: \$ 349,976; 09.01.2013-08.30.2018
21. Fundamentals of Adsorption, PI, NSF CBET (11551591), Award Amount: \$15,000; 10.01.2015 - 09.30.2016
22. Modeling of self-assembly and transport in polymer electrolyte membranes, PI, NSF DMR, Award Amount: \$383,803; 09.01.2012-08.31.2016
23. Computer laboratory for multi-scale simulations of novel nanomaterials, PI, DoD – DURIP (W911 NF-12-1-0328), Award Amount: \$ 99,924; 07.15.2012-07.14.2014.
24. Multiscale Modeling of Adsorption Equilibrium and Dynamics in Polymer Chromatography, PI, NSF, Award Amount: \$ 300,000; 04.15.2011-03.31.2016.

25. Molecular Design and Characterization of Novel Nanoporous Adsorbents with Increased Chemical Removal Capacity, PI, ARO, Award Amount: \$ 150,000; 06.15.2009-06.14.2011.
26. Adsorption-induced deformation of nanoporous materials, PI, Blaise Pascal International Chair Award, ENS Foundation, EUR 200,000; 09.01.09-08.31.11.
27. Adsorption and Chromatographic Separation of Chain Molecules on Nanoporous Substrates, PI, PRL-ACS, \$100,000, 01.01.09-08.31.11
28. Multiscale Modeling of Permeability of Protective Polyelectrolyte Membranes to CBW Agents, PI, DTRA (BRBAA07-F-2-0078); Award Amount: \$750,000; 07.01.08 – 06.30.12
29. Carbon Nanotube Fibers as Implantable Neural Electrodes, PI, NIH (R01 EB007467-01, subcontract to TRI); Award Amount: \$612,000; 09.01.07 - 08.30.11
30. Multiscale Modeling of Polymeric Systems, PI, Colgate Palmolive. Award Amount: \$275,000; 10.01.07 - 11.30.10
31. Computational System for Simulation of Nanostructured Polymeric Materials, PI, DURIP DOD (07030491). Award Amount: \$70,761; 04.18.07 - 04.17.08
32. Molecular Design of Sulfonated Tri-block Copolymer Permselective Membranes, PI, ARO (W911NS-07-1-0048); Award Amount: \$68,000; 12.07.06 - 12.06.07

**Multi-faculty programs:**

33. REU Site: Advanced Materials at Rutgers Engineering, NSF-DMR- 2149971, Award Amount: \$324,900, 01/01/2022 – 12/31/2025 (support of summer student)
34. REU Site: Advanced Materials at Rutgers Engineering, NSF-DMR-1659099, Award Amount: \$324,900, 05/01/2017 – 04/30/2020 (support of summer student)
35. GAANN graduate program on Pharmaceutical Engineering, Department of Education, Co-PI, Chair Student Review Committee, Award Amount: \$698,000; 09.01.09-08.31.14 (support for 3 years of PhD student),
36. Engineering Research Center (ERC) for Structured Organic Particulate Systems, NSF (0540855), Faculty member, support for 1 year of postdoc, 02.01.08-01.31.09.
37. IGERT: Nano-Pharmaceutical Engineering and Science NSF (0504497), Faculty member, support for 2 years of PhD student; 07.01.07 - 06.31.09.
38. Rutgers Catalyst Manufacturing Consortium (Faculty member), support for 0.5 PhD student; 10.01.07 - 09.30.09.

**LIST OF PUBLICATIONS**

**BOOK**

Kheifets L.I., Neimark A.V. Multiphase processes in porous media. Moscow: Khimia. 1982. 320p.

**EDITED VOLUMES**

11. Neimark A.V., Fomkin A.A., and Men'schikov I., Special issue dedicated to the 120th anniversary of Academician M.M. Dubinin, ADSORPTION, V. 29, Issues 5-6, 2023
10. Neimark A.V. and Thommes M., Characterization of porous materials: from Angstroms to millimeters – VIII, Microporous and Mesoporous Materials, V. 304, 2020
9. Neimark A.V. and Thommes M., Characterization of porous materials: from Angstroms to millimeters – VII, COLLOIDS AND SURFACES A, V. 496, 2016
8. Neimark A.V. and Thommes M., Characterization of porous materials: from Angstroms to millimeters – VI, COLLOIDS AND SURFACES A, V. 437, 2013
7. Neimark A.V. Characterization of porous materials: from Angstroms to millimeters - V COLLOIDS AND SURFACES A, V. 357 (1-3), 2010
6. Neimark A.V. Characterization of porous materials: from Angstroms to millimeters - IV COLLOIDS AND SURFACES A, V. 300 (1-2); 2007
5. Thommes M, Neimark A.V. Characterization of porous systems PARTICLE & PARTICLE SYSTEMS CHARACTERIZATION, V. 21 (2); 2004
4. Neimark A.V. Characterization of porous materials: from Angstroms to millimeters - III COLLOIDS AND SURFACES A, V. 241 (1-3); 2004
3. Neimark A.V. Nanocapillarity: Wetting of Heterogeneous Surfaces and Porous Solids. COLLOIDS AND SURFACES A, V. 206 (1-3); 2002
2. Neimark A.V. Characterization of Porous Materials: from Angstroms to millimeters – II. COLLOIDS AND SURFACES A, V. 187 (1-2); 2001
1. Neimark A.V. Characterization of porous materials: from angstroms to millimeters - I. ADVANCES IN COLLOID AND INTERFACE SCIENCE, V. 77 (1-2); 1998

## **INVENTIONS**

7. Colon, J.; Tsilomelekis, G; Neimark, A.V. “Method for detection of the Permeation of Chemical Warfare Agents through membranes”, - U.S. Patent Application 16/988,945, 08/10/2020
6. Landers, J.; Colon, J.; Goswami, A.; Asefa, T.; Vishnyakov, A.; Neimark, A.V. “Multicatalyst Polyelectrolyte Membranes and Materials and Methods Optimizing the Same”, - US Patent No. 10,722,743, 07/28/2020
5. Lewitus D., Landers J., Kohn J. and Neimark A.V., - Bioactive Carbon Nanotube - Agarose Composites for Neural Engineering. US patent application No US20120237557A1, 09/20/2012.
6. Neimark A.V., Kornev K.G., Bazilevsky A. V., and A.N. Rozhkov. - Light Beam Measurement of Absorption by Substrates. US patent No. US6731387B2,05/04/2004
3. Chesnokov B.B., Davidov V.A., Neimark A.V. et al. - A method of management for the process of granulation of powder materials. Authors certificate No. 1310015 of 15.01.87. Moscow.
2. Grinberg S.B., Kheifetz L.I., Neimark A.V. et al. - A catalyst for chlormetil synthesis. Authors certificate No. 1157739 of 22.01.85. Moscow
1. Bouden B.S., Kheifets L.I., Neimark A.V. et al. - A support of phosphoric acid catalyst for hydration of olephins. Authors certificate No. 750805 of 28.03.81. Moscow.

## **Published peer-reviewed papers (134 out of 291 total) published in 2006-2020 (at Rutgers); listed in reverse chronological order.**

### **2023**

291. Hough, Michael; Deditius, Artur; Robinson, Neil; Schröder-Turk, Gerd; Kirkensgaard, Jacob; Gun'ko, Volodymyr; Neimark, Alexander; Kaneko, Katsumi; Kowalczyk, Piotr, Ultrasonic spray nozzle-mediated green activation for hierarchical-pore structured carbon beads, ACS Sustainable Chemistry & Engineering, 2023, DOI: <https://doi.org/10.1021/acssuschemeng.3c04171>.
290. Fernando Vallejos-Burgos, Carla de Tomas, Nicholas J. Corrente, Koki Urita, Chiharu Urita, Shuwen Wang, Chris Chivers, Irene Soares-Martinez, Nigel A. Marks, Radovan Kukobat, Alexander V. Neimark, and Katsumi Kaneko, Realistic 3D Pore Size Distribution (3D-PSD) of Nanoporous Carbons, Carbon, 2023, 118431; DOI: <https://doi.org/10.1016/j.carbon.2023.118431>.
289. Kolattukudy P. Santo, Alexander Neimark, Adsorption of Pulmonary and Exogeneous Surfactants on SARS-CoV-2 Spike Protein, Journal of Colloid and Interface Science, 2023, V. 578, p.28-39; DOI: <https://doi.org/10.1016/j.jcis.2023.06.121>.

### **2022**

288. Shivam Parashar, Peter I. Ravikovitch, and Alexander V. Neimark, Molecular modeling and adsorption characterization of micro-mesoporous kerogen nanostructures, ACS Energy & Fuels, 2022, V.36, p.13037-13076. DOI: <https://doi.org/10.1021/acs.energyfuels.2c02876>.
287. Bartosz Mazur, Filip Formalik, Kornel Roztocki, Volodymyr Bon, Stefan Kaskel, Alexander V. Neimark, Lucyna Firlej, Bogdan Kuchta, Quasi-continuous cooperative adsorption mechanism in crystalline nano-porous materials, JPC Letters, 2022, V. 13, p. 6961-6965. DOI: [10.1021/acs.jpcclett.2c01752](https://doi.org/10.1021/acs.jpcclett.2c01752).
286. Piotr Kowalczyk, Artur P. Terzyk, Paulina Erwardt, Michael Hough, Artur Deditius, Piotr A. Gauden, Alexander V. Neimark, and Katsumi Kaneko, Machine learning-assisted design of porous carbons for paracetamol removal from aqueous solutions, Carbon, 2022, V.198, p. 371-381. DOI: [/10.1016/j.carbon.2022.07.029](https://doi.org/10.1016/j.carbon.2022.07.029).
285. Nicholas J. Corrente, Elizabeth L. Hinks, Aastha Kasera, Peter I. Ravikovitch, and Alexander V. Neimark, Modeling Hydrocarbons Adsorption in Amorphous Nanoporous Carbonaceous Materials, Carbon, Carbon, 2022, V.197, p.526-533. DOI: [10.1016/j.carbon.2022.06.071](https://doi.org/10.1016/j.carbon.2022.06.071) chemRxiv, 05/25/2022; DOI: <https://doi.org/10.26434/chemrxiv-2022-fs4kr>.

### **2021**

284. Aleksey Vishnyakov, Runfang Mao, Kimberly Kam, Alexander V Neimark, Interactions of polyelectrolyte gels with nonionic and ionic surfactants, Journal of Physical Chemistry B, 2021, V.125, p. 13817–13828, DOI: [/10.1021/acs.jpcc.1c08638](https://doi.org/10.1021/acs.jpcc.1c08638).
283. Kolattukudy P. Santo and Alexander V. Neimark, Dissipative Particle Dynamics Simulations in Colloid and Interface Science: A Review, Advances in Colloid and Interface Science, 2021, V.298, 1025545, DOI: [10.1016/j.cis.2021.102545](https://doi.org/10.1016/j.cis.2021.102545).
282. Nicholas J. Corrente, Katarzyna Zarebska, and Alexander V. Neimark, Deformation of Nanoporous Materials in the Process of Binary Adsorption: Methane Displacement by Carbon Dioxide from Coal, J. Physical Chemistry C, 2021, V.125, P. 21310-21316, DOI: [10.1021/acs.jpcc.1c07363](https://doi.org/10.1021/acs.jpcc.1c07363).

281. Kolattukudy P. Santo, Kristina I. Fabijanic, Chi-Yuan Cheng, Andrei Potanin, and Alexander V. Neimark, Modeling of the effects of metal-complexation on morphology and rheology of Xanthan Gum polysaccharide solutions, *Macromolecules*, 2021, V. 54, p. 8675-8692, DOI: 10.1021/acs.macromol.1c01328.
280. S.M.P. Lucena, J.C.A. Oliveira, D.V. Gonçalves, P.F.G. Silvino, S. Dantas, and A.V. Neimark, Pore size analysis of carbons with heterogeneous kernels from reactive molecular dynamics model and quenched solid density functional theory. *Carbon*, 2021, V. 183, p.672-684, DOI: 10.1016/j.carbon.2021.07.05.
279. Kolattukudy P. Santo and Alexander V. Neimark, Effects of Metal-Polymer Complexation on Structure and Transport Properties of Metal-Substituted Polyelectrolyte Membranes, *Journal of Colloid and Interface Science*, 2021, V.602, p.654-668, DOI: 10.1016/j.jcis.2021.06.018.
278. Shivam Parashar, Qing Zhu, Silvio Dantas, and Alexander V. Neimark, Compartmentalization of Adsorption Isotherms Reveals the Specifics of Guest-Host Interactions. *ACS Appl. Nano Mater.*, 2021, V.4, p. 5531-5540, DOI: 10.1021/acsanm.1c00937.
277. Anton A. Belogorlov, Vladimir D. Borman, Igor A. Khlistunov, Vladimir N. Tronin, and Alexander V. Neimark, Suspensions of Lyophobic Nanoporous Particles as Smart Materials for Energy Absorption, *Journal of Colloid and Interface Science*, 2021, V.600, p. 229-242. DOI: 10.1016/j.jcis.2021.04.132.
276. Silvio Dantas, Katie Cychosz, Matthias Thommes, and Alexander V. Neimark, Monte Carlo simulation method for calculating pore size distributions from high-pressure CO<sub>2</sub> adsorption in Micro-Mesoporous Carbons, *Carbon*, 2021, V.173, P.842-848. DOI: 10.1016/j.carbon.2021.01.059.
275. Parva Patel, Kolattukudy P. Santo, Sean Burgess, Aleksey Vishnyakov, and Alexander V. Neimark, Stability of Lipid Coatings of Nanoparticle Decorated Surfaces, *ACS Nano*, 2020, V.14, P.17273-117284; DOI: 10.1021/acsnano.0c07298.
274. Xinyang Wang, Kolattukudy P. Santo, and Alexander V. Neimark, Modeling Gas-Liquid Interfaces by Dissipative Particle Dynamics: Adsorption and Surface Tension of Cetyl Trimethyl Ammonium Bromide at Air-Water Interface, *Langmuir*, 2020, V.36, 14686-14698. DOI: 10.1021/acs.langmuir.0c02572.
273. Piotr Kowalczyk, Yasunori Yoshikawa, Katsuya Teshima, Ryusuke Futamura, Hideki Tanaka, Alexander V. Neimark, and Katsumi Kaneko, Structural mechanism of reactivation with steam of pitch-based activated carbon fibers, *Journal of Colloid and Interface Science*, 2020, V. 578, p.422-430; DOI: 10.1016/j.jcis.2020.06.002.
272. Filip Formalik, Justyna Rogacka, Lucyna Firley, Bogdan Kuchta, and Alexander V. Neimark, Gate Opening and Breathing Transitions in Metal-Organic Frameworks: Coupling Adsorption and Deformation, *Journal of Colloid and Interface Science*, 2020, V. 578, p. 77-88; DOI: 10.1016/j.jcis.2020.05.105.
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171. A. Vishnyakov and A.V. Neimark, - Molecular Simulation Study of Sulfonated Polystyrene Solvation in Polar Solvents: Water and Dimethylmethylphosphonate, - *Journal of Chemical Physics*, 2008, V. 128, 164902.
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## 2007

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163. P.I. Ravikovitch and A. V. Neimark, - Density Functional Theory Model of Adsorption Deformation – *Langmuir*, 2006, V.22, 11171-11179.
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161. A. V. Neimark and A. Vishnyakov, - Phase transitions and criticality in small systems: vapor-liquid transition in nanoscale spherical cavities. - *Journal of Physical Chemistry*, 2006, V.110, p.p.9403-9412.
160. P.I. Ravikovitch, A. Vishnyakov, A.V. Neimark, M.R. Carrott, P.A. Russo, P.J. Carrott. - Characterization of Micro-Mesoporous Materials from Nitrogen and Toluene Adsorption: Experiment and Modeling, - *Langmuir*, 2006, V.22, p.p.513 -516.
159. P.I. Ravikovitch and A. V. Neimark. - Density Functional Theory Model of Adsorption on Amorphous and Microporous Solids - *Studies in Surf. Sci. & Catal.*, 2006, pp. 9-16.
158. M. Thommes, B. Smarsly, M. Groenewolt, P.I. Ravikovitch, A.V. Neimark.- Adsorption Hysteresis of Nitrogen and Argon in Pore Networks and Characterization of Novel Micro-Mesoporous Silicas. – *Langmuir*, 2006, V. 22, p.p. 756-764.

## **INVITED LECTURES AND SEMINARS, KEYNOTE & PLENARY TALKS, 2006-2017 (at RUTGERS)**

### **2023**

- Invited talk, 3D Molecular Models of Disordered Carbons for Pore Structure Characterization and Predicting Adsorption and Mechanical Properties, Symposium on Challenges for Carbon- based Nanoporous Materials (7CBNM) in Nagano, Japan
- Invited seminar on “Competitive Adsorption of Surfactants and Amino Acids on Dental Biofilms: Insight from Multiscale Molecular Simulations”, Tech Exchange Meeting at Colgate-Palmolive, Piscataway, NJ
- Invited seminar “Interactions of Coronavirus Virions as Biological Nanoparticles with Respiratory Environment: Insight from Multiscale Molecular Simulations”, Thomas Young Center, Imperial College, London, UK.
- Invited seminar, Recent Advances in Characterization of Structural and Adsorption Properties of Nanoporous Carbons, Tohoku University, Sendai, Japan
- Invited seminar, Alexander V. Neimark, Novel Approach to Advanced Adsorption Characterization of Pore Structure of Metal-Organic Frameworks. Kyoto University, Japan

### **2022**

- Keynote lecture. Coarse-Grained Simulations of Interactions of Nanoparticles with Soft Interfaces. 2022 NJIT Molecular Simulations Workshop, NJIT, NJ
- Keynote Invited Talk “Dissipative Particle Dynamics of Soft Matter Systems”, 11<sup>th</sup> International Colloids Conference, Lisbon, Portugal, 12-15 June 2022
- Invited Talk “Mesocanonical Ensemble as a Rational to Study Fluctuations and Phase Transformations in Nanoconfined Fluids.” Venice Meeting on Fluctuations in Small Complex Systems VI. Venice Italy
- Invited Plenary Talk “Selective Adsorption of Surfactants on Coronavirus Virions”. The 2022 AIChE Annual Meeting, Fenix, Arizona
- Invited Seminar. Modeling of Nanoparticle Interactions with Soft Interfaces. University of California, Riverside, California
- Adsorption Characterization of MOF Materials: Real Samples vs Ideal Crystals. International Adsorption Society Webinar Series

### **2021**

- Invited Plenary Lecture, “Thermodynamics of Adsorption Deformation of Microporous Carbons”, Russian Conference “Physicochemical Problems of Adsorption, Structure and Surface Chemistry of Nanoporous Materials” in honor of M.M. Dubinin, Moscow, Russia
- Invited Seminar "Mesoscale Modeling of Soft Matter Systems", Chimie ParisTech, Paris, France
- Navier seminar “Multiscale Nature of Poromechanics of Nanoporous Adsorbents”, Ecole des Ponts ParisTech, Champs-sur-Marne, France

- Thermodynamics of Adsorption-induced Deformation of Nanoporous Solids: Old Problem, Enigmatic Features, and Modern Applications, ATOMS seminar series, Federal University of Rio de Janeiro, Brazil.
- Morgan Advanced Materials Lecture, “Recent Advances in Characterization of Structural and Adsorption Properties of Nanoporous Carbons”, PennState, PA

## 2020

- Invited seminar “Morphology, Rheology, and Transport Properties of Surfactant and Polymeric Solutions: Insight from Dissipative Particle Dynamics Simulations” at International Flavors and Fragrance (IFF) company:

## 2019

- Invited Seminars in Japan:
  - Matsumoto University, March 8
  - Waseda University, Tokio, March 11
  - Kanazawa University, March 13
- Lecture Series “Advanced Methods for Modeling and Characterization of Nanoporous Materials”, Shinshu University, Nagano, Japan, March 6-22
- Keynote Lecture, “Adsorption Induced Deformation of Hierarchical Micro-Mesoporous Materials”, 13<sup>th</sup> International Conference on the Fundamentals of Adsorption, Cairns, Australia, May 26-31.
- Tutorial Lecture “Modern Advances on Pore Structure Characterization”, 13<sup>th</sup> International Conference on the Fundamentals of Adsorption, Cairns, Australia, May 26-31.
- Plenary Lecture “Adsorption Induced Deformation and Phase Transformations in Nanoporous Crystals”, International Conference "Mechanisms and Non-Linear Problems of Nucleation and Growth of Crystals and Thin Films", St. Petersburg, Russia, July 1-5.
- Invited Seminar, Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow, Russia, July 9.
- Invited Seminar, Imperial College London, UK, July 15.
- Thomas Young Centre Soiree Lecture “Breathing Solids: Adsorption-Induced Deformation of Nanoporous Materials”, Queen Mary University of London, UK, July 18.
- Leverhulme Lecture “Recent Advances in Structure Characterization of Nanoporous Materials”, University College London, UK, July 24.
- Invited Lecturer, 1<sup>st</sup> International Gas Adsorption Summer School, Spetses, Greece, September 9-14.
- Invited Seminar, Flow, Adhesion, and Separation of Functionalized Nanoparticles on Porous Substrates, Exxon-Mobil research and Engineering, Annandale, NJ, September 23.
- Claude R. Hocott Lecture in Petroleum Engineering, University of Texas in Austin, October 14.
- Invited talk “Adsorption Stress as a Rational for Quantification of Host-Guest Mechanical Interactions in MOFs and Other Nanoporous Materials”, FlexMOF Symposium, December 3-5, Dresden, Germany.

## 2018

- Invited Lecture “DPD Modeling of Phase Segregation, Diffusion, and Conductivity in Polyelectrolyte Membranes”. CECAM Workshop “Dissipative Particle Dynamics: Where do we stand on predictive applications? Daresbury Laboratory, Manchester, UK, April 24-26.
- Invited Talk. “Breathing Solids: from Human Hair to Designer Nanoporous Materials”, Engineering Department Bio- and Micromechanics Seminars, Cambridge University, UK, June 8.
- Leverhulme Lecture Series
  - University College London, UK, June 27.
  - University of Manchester, UK, June 28.
  - University of Bath, UK, July 5.
  - University of Edinburgh, UK, July 12.
  - University College London, UK, October 24.
- Lecture Series “Advanced Methods for Modeling and Characterization of Nanoporous Materials”, Shinshu University, Nagano, Japan, Aug. 29 -Sept. 11, 2018.
- Invited Plenary Talk “Size-Independent Separation of Functionalized Nanoparticles on Porous Substrates”, AIChE Annual Meeting, Pittsburg, PA, Oct. 28-Nov. 2.

## 2017

- Invited Seminar “From Multiscale Modeling of Self-Assembly in Polyelectrolyte Membranes to Fabrication of Multicatalyst Composite Barriers”, Department of Chemical and Biological Engineering, South Dakota School of Mines and Technology, Rapid City, South Dakota,
- Invited Talk. “Self-Assembly and Transport in Polyelectrolyte Membranes”, Aleksey Vishnyakov, Ming-Tsung Lee, and Alexander V. Neimark, 2017 MRS Spring Meeting, Symposium: CM3: Computer-Based Modeling and Experiment for the Design of Soft Materials, Phoenix, Arizona, April 17-21, 2017.
- Invited Seminar. Self-Assembly and Transport in Polyelectrolyte Membranes. University Pierre and Mary Curie, Paris, France, May 5, 2017.
- Invited Talk. 9th International Conference on Porous Media & Annual Meeting Minisymposium "Fluids in Nanoporous Media", Rotterdam, The Netherlands, May 8-11, 2017.
- Invited lecture “Multiscale Modeling of Water and Proton Diffusion in Self-Assembled Polymer Electrolyte Membrane”, Aleksey Vishnyakov, Ming-Tsung Lee, and Alexander V. Neimark. VII International Conference “Diffusion Fundamental”, July 3-7, Moscow, Russia.
- Invited Seminar “Self-Assembly and Transport in Polyelectrolyte Membranes: from Multiscale Modeling to Design of Novel Materials”, National Research Nuclear University MEPhI, Moscow, Russia, July 6, 2017.
- Plenary Lecture “Reconciliation of Gibbs excess adsorption thermodynamics and poromechanics of nanoporous materials” 6th Biot Conference on Poromechanics, 9-13 Jul 2017, Paris, France.
- Invited Lecture “Adsorption Deformation from the Position of Poromechanics”, Workshop on DIANA project, Leoben, Austria, Jul.17, 2017.
- Keynote Talk “Thermodynamics and Transport in Self-Assembled Polyelectrolyte Membranes “, 9<sup>th</sup> Sino-US Joint Conference of Chemical Engineering, Beijing, China, October 16, 2017
- Invited Seminar. Beijing University of Chemical technology, Beijing, China, October 16, 2017
- Invited Lecture. “Frontiers of Materials Science”, University of Chinese Academy of Science, Huairou, Beijing, China, October 17, 2017
- Invited Seminar. Peking University, Beijing, China, October 19, 2017
- Invited Seminar. Soft Matter Center, Beihang University, Beijing, China, October 19, 2017

## 2016

- Invited Seminar “Coarse-grained Modeling of Self-Assembly and Transport in Polyelectrolyte Membrane”, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC, March 2, 2016.
- Invited seminar “Multiscale Modeling of Chain Molecules: from Self-Assembly in Surfactant Solutions to Grafted Surfaces to Polymer Chromatography”, ExxonMobil Research and Engineering Company, Annandale, NJ, April 6, 2016
- Colloquium of the International Graduate Research Training Group, Technical University, Berlin, Germany, May 23-28, 2016.
- Plenary Tutorial Lecture “Recent Advances in Molecular Simulation of Adsorption”, 12<sup>th</sup> International Conference on Fundamentals of Adsorption (FOA12), Friedrichshafen, Germany, May 29 - June 3, 2016.
- Plenary Lecture. “Adsorption Deformation of Nanoporous Materials: from Single Crystals to Hierarchical Structures”, 40th Reunião Ibérica de Adsorção (RIA 2016), Evora, Portugal, September 5-7, 2016.
- Plenary talk “Adsorption Stress in Nanopores”, AIChE Annual Meeting, San Francisco, CA, Nov. 13-8, 2016.

## 2015

- Invited seminar “Poromechanics of Adsorbents”, ExxonMobil Research and Engineering Company, Annandale, NJ, January 6, 2015.
- Invited Speaker. The Fourth Symposium on Challenges for Carbon-based Nanoporous Materials: Adsorption and Energy, Nagano, Japan, March 16-18, 2015.
- Invited Lecturer. “Advances in the Density Functional Theory for Characterization of Porous Solids”. II Latin American Congress of Adsorption and The Second School Giorgio Zgrablich, Cartagena de Indias, Colombia, April 26-30, 2015.
- Invited Talk. “Self-Assembly, Transport, and Thermodynamics in Nafion membranes: Insight from Dissipative Particle Dynamics Simulation”, Aleksey Vishnyakov, Ming-Tsung Lee, and Alexander V. Neimark , 227<sup>th</sup> Annual Meeting of the Electrochemical Society, Symposium L3, Chicago, Illinois, May 24-28, 2015.
- Invited Seminar. University of Southern California, June 18, 2015.

- Showcase talk. “Studies of Nanoparticle Adhesion to Soft Interfaces and Membranes by the Ghost Tweezers Method”, Jianli Cheng, Zhenjia Wang, Sean Burgess, Aleksey Vishnyakov, and Alexander V. Neimark. 5<sup>th</sup> International Colloids Conference, Amsterdam, June 21-24, 2015.
- Invited Talk. “Ghost Tweezers Method for Studies of Nanoparticle Interactions with Soft Interfaces”, Jianli Cheng, Zhenjia Wang, Sean Burgess, Aleksey Vishnyakov, and Alexander V. Neimark, Symposium "Theory and Modeling of Nanoparticle Interactions with Biomolecules and Polymers", ACS Fall National Meeting, Boston, MA, August 16-20, 2015.
- Invited Speaker. Bishop Advanced Materials Colloquium Series, Clemson University, September 18, 2015.
- Invited Seminar. East China University of Science and Technology, October 12, 2015, Shanghai, China.
- Keynote Speaker. Thermodynamics of Deformation and Phase Transformations in Nanoporous Adsorbents, 8th Sino-US Joint Conference of Chemical Engineering, Shanghai, China, October 12-15, 2015.
- Plenary talk. Critical Conditions of Polymer Chromatography on Nonporous Substrates, Richard T. Cimino, Christopher J. Rasmussen, Yefim Brun and Alexander V. Neimark. International Symposium on GPC/SEC and Related techniques, Philadelphia, October 20-22, 2015.
- Invited Talk. “Solvation-Induced Self-Assembly of Polyelectrolyte Membranes”, Aleksey Vishnyakov, Ming-Tsung Lee, and Alexander V. Neimark, International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 15-20, 2015.

## 2014

- Invited speaker. CECAM workshop “Dissipative Particle Dynamics: Foundations to Applications”, Lausanne, Switzerland, May 7-9 May, 2014.
- Plenary talk. The 10th International Symposium on the Characterization of Porous Solids (COPS-X), Granada, Spain, May 11-14, 2014.
- Invited speaker. The 13th International Ceramics Congress, Symposium CH “Porous Ceramics for Environmental Protection, Energy-related Technologies and Advanced Industrial Cycles”, Montecatini Terme, Tuscany, Italy, June 8-13, 2014.
- Invited lecture “Quenched Solid Density Functional Theory of Adsorption on Heterogeneous Solids and Pore Structure Characterization”, Workshop “Characterization of Nanoporous Materials: Correlating Textural Properties to Applications in Gas and Energy Storage, Separation, and Catalysis”, Stanford University, August 8-9th, 2014.
- Invited speaker “Studies of Nanoparticle Adhesion to Soft Interfaces and Membranes by the Ghost Tweezers Method”, Jianli Cheng, Zhenjia Wang, Aleksey Vishnyakov, and Alexander V. Neimark, CECAM-COST Workshop “Friction and Interface Dynamics at Nano and Mesoscales”, Tel-Aviv, Israel, October 27 -31, 2014.
- Invited Speaker. NIST/CCR workshop on “Measurement Needs in the Adsorption Sciences”, Gaithersburg, MD, November 5-6, 2014
- Invited Seminar. “Self-Assembly in Surfactant and Polymeric Systems: Insight from Dissipative Particle Dynamics Simulations” Department of Chemistry, University of Georgia, Athens, GA, November 21, 2014.

## 2013

- Invited lecture “Revisiting Percolation Models of Capillary Hysteresis”, Giorgio Zgrablich” School on Adsorption, Adsorbents and their Applications, San Luis, Argentina, February 18-21, 2013.
- Invited seminar, Department of Chemical Engineering and Materials Science at the University of Southern California, Los Angeles, CA, April 1, 2013.
- Invited lecture “Deformation of Adsorbents”, Federal University of Ceara, Fortaleza, Brazil, May 3, 2013.
- Plenary talk “Modeling adsorption effects of complex polymers in solvent-gradient interaction chromatography”, Christopher J. Rasmussen (presenter), Yefim Brun, and Alexander V. Neimark, 11th International Conference on the Fundamentals of Adsorption Baltimore, Maryland, USA, May 19-24, 2013
- Plenary talk “Deformation of Mesoporous Silica upon n-Pentane Adsorption: Verifying Theory Against SAXS”, Gennady Gor (presenter), Oskar Paris, Johannes Prass, and Alexander V. Neimark, 11th International Conference on the Fundamentals of Adsorption Baltimore, Maryland, USA, May 19-24, 2013
- Invited lecture “Adsorption on compliant porous materials”, II Workshop on Adsorption, Bogota, Colombia, May 27-31, 2013

- Invited lecture “The affect of surface roughness on the structure and properties of confined fluids: quenched-solid density functional theory”, CECAM workshop "New Perspectives in Liquid State Theories for Application to Complex Molecular Systems", Paris, France, June 20-22, 2013
- Invited lecture “Interplay of capillary and disjoining pressures during condensation-evaporation cycles in mesoporous solids”, Workshop on "Strains induced by phase changes in deformable porous solids", Ecole des Ponts ParisTech, France, July 8-9, 2013
- Keynote talk “Found in Translation: from Thermodynamics of Adsorption to Poromechanics of Nanostructure Solids”, Minisymposium on “Microporous and mesoporous materials: adsorption and poromechanics”, 5<sup>th</sup> Biot Conference on Poromechanics, Vienna, Austria, July 10-12, 2013
- Invited talk, “Adsorption induced deformation and phase transformations of microporous and mesoporous crystals”, International Porous and Powder Materials Symposium, PPM-2013, Izmir, Turkey, Sept. 3-6, 2013
- Invited Seminar “Self-Assembly and Transport in Soft Nanomaterials: Insight from DPD modeling”, Physics Department, University of Southern California, Los Angeles, CA, Sept. 20, 2013.
- Invited seminar, Department of Chemical Engineering, University College London, UK, Oct.2, 2013.
- Invited seminar, Department of Chemical Engineering, Imperial College London, UK, Oct.15, 2013.
- Invited seminar, School of Chemical Engineering and Analytical Sciences University of Manchester, UK, Oct. 23, 2013
- Tomas Young Center Soiree Lecture “Self-Assembly and Transport in Soft Nanomaterials: Insight from DPD modeling”, King’s College, London, UK, Oct. 24, 2013.
- Invited seminar, Department of Chemistry, Imperial College London, UK, Oct.29, 2013.
- Invited talk, “QSDFT Model for Simulation of Adsorption Isotherms and Characterization of Adsorbents”, Industrial Fluid Properties Simulation Challenge session, Annual AIChE Meeting, San Francisco, November 4-8, 2013.

## 2012

- Invited Plenary Talk. Theoretical and Experimental Studies of Scanning Isotherms, Alexander V. Neimark, Richard Cimino, Katie A. Cychoz, and Matthias Thommes, Session in honor of Gino Baron, Annual AIChE Meeting, Pittsburgh, October 28- November 2, 2012
- Invited Talk. Scanning Adsorption-Desorption Hysteresis, Alexander V. Neimark, Richard Cimino, Katie A. Cychoz, and Matthias Thommes, 8<sup>th</sup> International Symposium of Surface heterogeneity in Adsorption and Catalysis on Solids, ISSHAC-8, Krakow, Poland, August 27-31.
- Keynote lecture. International Symposium on Zeolites and Microporous Materials (ZMPC-2012), Hiroshima, Japan, July 28 – August 1, 2012.
- Invited Seminar. Ecole Normale Supérieure, Paris, France, June 22, 2012.
- Blaise Pascal Lecture, Chimie ParisTech, Paris, France, June 12, 2012.
- Keynote lecture. Percolation and Fractal Models of Capillary Phenomena in Pore Networks, PEDOFRACT Workshop, La Coruna, Spain, May 14-17, 2012.
- Invited lecture. Breathing Transitions in MOF. The 1st Ibero-American Symposium on Adsorption (IBA-1), Recife, Brazil, May 6- 10, 2012.
- Invited Seminar. Department of Chemistry, City College, CUNY, New York, NY, March 26, 2012.
- Invited Lecture. Modeling Adsorption and Translocation of Chain Molecules in Nanopores, Nanopore Conference, Puerto Calero, Spain, Feb. 6-10, 2012.

## 2011

- Breathing Crystals: Adsorption Deformation and Structural Transitions in Metal-Organic Frameworks, Invited Talk, Statistical-Mechanical Conference, Rutgers, Dec. 18-20, 2011.
- Seminar at Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia, October 28, 2011
- Deformation of Micro- and Mesoporous Adsorbents, Invited lecture, International Conference on Modern Problems of Adsorption, Moscow, Russia, October 26, 2011
- Adsorption Deformation of Porous Materials: from MMC to MOF, Plenary lecture, AIChE Meeting, Minneapolis, October 17-20, 2011.
- Breathing Crystals: Adsorption Deformation and Structural Transitions in Metal-Organic Frameworks, Seminar at PRISM, Princeton University, October 12, 2011.
- Seminar at Department of Chemistry, Peking University, Beijing, China, September 30, 2011
- Seminar at Department of Chemical Engineering, Beijing University of Chemical Technology, China, September 28, 2011



- Seminar at Department of Chemical Engineering, Tsinghua University, Beijing, China, September 27, 2011
  - Invited lecture series at Nanjing University, China, September 19-23, 2011
  - Multiscale Modeling of Permeability of Protective Polyelectrolyte Membranes to CBW Agents, Invited talk, DTRA Multifunctional Materials Workshop, Natick, MA, August 21, 2011.
  - Characterization of Carbons with Ordered Spherical Mesopores by High Resolution Sorption and Hysteresis Scanning Experiments in Combination with Novel QSDFT Methods. Keynote talk. Katie A. Cychoz, X. Guo, Gennady Gor, Wei Fan, Alexander V. Neimark, Matthias Thommes (presenter), Michael Tsapatsis, International Carbon Conference, Shanghai, China, July 24-26, 2011.
  - Adsorption deformation: What we want to understand? Opening lecture, CNRS Workshop "Adsorption in Compliant Solids: Theory, Simulation, and Experiments", June 9-11, Paris, France Paris.
  - Invited Lecture. Symposium in honor of Katsumi Kaneko, University Pierre and Marie Curie, Paris, June 13, 2011.
  - Structural transitions in MOF: view from outside and inside [Alexander V. Neimark](#), F.-X. Coudert, C. Triguero, A. Boutin, A.H. Fuchs, I. Beurroies, and R. Denoyel, 9th International Symposium on Characterization of Porous Solids (COPS-9), Dresden, June 5-8, 2011.
  - Density Functional Theory of Inhomogeneous Fluids: Bridging Scales from Molecular Simulations to Macroscopic Description. Invited Lecture. Journées Modélisation de Paris, ENS, Paris, France, May 18, 2011.
  - Lecture at the Rutgers Catalysts Roadshow at BASF Catalysts, Iselin, NJ, May 10, 2011.
- 2010**
- Invited talk "Mesoscale simulation of nanosegregation in permselective polyelectrolyte membranes" with A. Vishnyakov (presenter) at the 239th ACS National Meeting, San Francisco, CA, March 21–25, 2010.
  - Plenary talk "The Role of Cavitation in Adsorption Hysteresis" with Christopher Rasmussen, Aleksey Vishnyakov, Matthias Thommes, Bernd Smarsly, and Freddy Kleitz, 10th International Conference on Fundamentals of Adsorption, Hyogo, Japan, May 23-28, 2010.
  - Invited talk "Solvation pressure between molecularly rough surfaces" at the ACS Symposium in honor of Dr Kash Mittal at the 240th ACS National Meeting, Boston, MA, August 23, 2010.
  - Invited seminar at the Laboratoire Chimie Provence, Universités d'Aix-Marseille, France, September 24, 2010.
  - Plenary talk " Adsorption-Induced Deformation of Nanoporous Materials: From MMS to MOF", with Yangzheng Lin, Yang Kan, Gennady Gor, François-Xavier Coudert, Anne Boutin and Alain H. Fuchs, AIChE annual meeting, Salt Lake City, UT, November 9-12, 2010.
  - Invited talk "Consistent Approach to Multiscale Simulations of Polyelectrolytes Using Dissipative Particle Dynamics" with A. Vishnyakov (presenter) at the 8th International Symposium on Polyelectrolytes, Shanghai, China, November, 16-18, 2010
  - Invited seminar at the Imperial College, London, UK, November 18, 2010.
- 2009**
- Seminar at the Institute Charles Gerhardt, Montpellier, France, December 10, 2009.
  - Adsorption and Translocation of Chain Molecules in Nanopores. Invited talk with Shuang Yang, Yang Kan, and Aleksey Vishnyakov, Fall Meeting of Materials Research Society, Boston, MA. December 3, 2009.
  - Seminar at the Ecole Polytechnique, Palaiseau, France. November 26, 2009.
  - Seminar at the Vrije Universiteit in Brussel, Belgium. November 24, 2009.
  - Blaise Pascal seminar at the Ecole Nationale Supérieure de Chimie de Paris, France. November 5, 2009.
  - Quenched Solid Density Functional Theory of Adsorption of Molecularly Rough Surfaces. Invited lecture. CECAM workshop "Classical Density Functional Theory Methods in Soft and Hard Matter" in Lausanne, Switzerland. October 21-23, 2009.
  - Invited lecture. Conference "Diffusion Fundamentals III", Athens, Greece. August 23-26, 2009.
  - Seminar at the Quantachrome Instruments, Boynton Beach, FL, February 8, 2009.
- 2008**
- Seminar at the US Army Research, Development and Engineering Command, Natick, Ma, December 8, 2008.
  - Adsorption on Molecularly Rough Surfaces, Plenary Session on Fundamentals of Adsorption and Ion Exchange, AIChE meeting, Philadelphia, November 16-21, 2008.

- The density functional theory of adsorption in pores: applications to advanced characterization of nanoporous materials. Invited Lecture. 1st International Workshop Nano-Porous Materials in Energy and Environment, Chania, Crete, Greece, October 12- 15, 2008
- Seminar at the Department of Chemistry, CSI, City University of New York, October 7, 2008
- Molecular Models for Adsorption and XRD Characterization of Templated Porous Materials. Invited Talk, CECAM workshop “Surfactant Templated Porous Materials: Synthesis and Characterization”, Zurich, Switzerland, September 10-12, 2008
- The Role of Surface Roughness in Adsorption: Applications to Nanoporous Carbons, invited talk at the International Workshop “Future Challenges for Carbon-Based Nanoporous Materials”, Chiba, Japan, July 11-13, 2008
- Recent Advances in Characterization of Nanoporous Materials, Invited Lecture on at the National Institute for Materials Science, Tsukuba, July 16, 2008
- Multiscale simulation of self-assembled polyelectrolyte membranes, with Aleksey Vishnyakov, Invited Lecture, 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), Vancouver, Canada, July 19-24, 2008.
- Multiscale simulation of self-assembled polyelectrolyte membranes, Invited lecture, 7th International Symposium on Polyelectrolytes, Coimbra, Portugal, June 16-19, 2008
- Seminar in the Department of Materials Science, Drexel University, Philadelphia, PA, May 12, 2008.
- Seminar in the Arrhenius Laboratory of Stockholm University, Stockholm, Sweden, May 5, 2008.

## 2007

- Fluid-Solid Interactions: Accounting for the Surface Roughness, Invited talk, the 98<sup>th</sup> Statistical Mechanics Conference, Rutgers, December 16-18, 2007.
- Mesoscopic Canonical Ensemble, Invited talk, International Conference “Thermodynamics 2007, Rueil-Malmaison, France, September 26 – 28, 2007.
- Application of a Novel Density Functional Theory to the Pore Size Analysis of Micro/Mesoporous Carbons, Keynote at the International Carbon Conference, Seattle, July 15-20, 2007 (with M. Thommes and P.I.Ravikovitch).
- Seminar at the Department of Chemical Technology, Delft University, Netherlands, November 23, 2007.
- Materials Science and Engineering Seminar, Rutgers University, Piscataway, NJ, October 30, 2007.
- Multiscale Modeling of Self-Assembled Polymeric Systems. Seminar at Colgate-Palmolive, Piscataway, NJ, June 14, 2007.
- Seminar at the US Army Research, Development and Engineering Command, Natick, Ma, May 15, 2007.

## 2006

- Invited Lecture. International Conference "Transport in polymeric membranes: modern trends in simulation methods and experimental techniques", Pula, Italy, October 15 – 18, 2006.
- Plenary talk. Formation and Characterization of Pore Structure in Carbon Nanotube Fibers. G. C. Callegari, K. G. Kornev, J. Kuppler, S. B. Ruetsch, A. V. Neimark. 5th International Mesostructured Materials Symposium, Shanghai, China, August 5-7, 2006.
- Invited Speaker. Density Functional Theory of Adsorption of Rough and Microporous Surfaces. 6th International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Zakopane, Poland, August 28 - September 2, 2006.
- Invited Lecture. Pre-school “Fundamental Practices of Mesostructured Materials”, Fudan University, Shanghai, China, Aug. 3-4, 2006.