Full list of Talks and Presentations

Usage, Dublin, Irelandinvited talk.

- June 2017 International Meeting on Atomic and Molecular Physics and Chemistry, Toruń, Poland, invited talk.
- April 2017 World Congress and Expo on Nanotechnology and Materials Science, Barcelona, Spain, invited talk.
- April 2017 International Workshop on Quantum Atomic and Molecular Tunneling in Solids and other Phases, Madison Wisconsin, USA, invited talk.
- February 2017 Seminar Series, Atomistic Simulation Center, Queen's University, Belfast, United Kingdom, **invited** seminar.
- November 2016 Theoretical Chemistry Informal Seminars Series, Department of Chemistry, University of Cambridge, United Kingdom.

 Invited Seminar: Predictive Multiscale Modelling: Multidisciplinary Challenges for
- the Future of Computational Chemistry

 September 2016 CECAM Workshop on Multiscale Simulation: from Materials Through to Industrial
 - **Contributed** Talk: Predictive Multiscale Modelling in Chemical Sciences: Interdisciplinary Challenges from a Multidisciplinary View Point
 - June 2016 Conference on 'Energy Landscapes: Theory and Applications', Centre IGESA, Porquerolles, France.
 - **Contributed** Talk: Kinetics of Molecular Diffusion and Self-Assembly: Glycine on Cu110.
 - Mai 2016 University of Munich, Department of Physics, Prof. Martin Zacharias, Munich, Germany.
 - **Invited** Seminar: An Interdisciplinary Perspective on Predictive Multi-scale Modelling and the Chemisorption of Glycine on Cu(110).
 - Mai 2016 University of Braunschweig, Department of Chemistry, Prof. Christoph Jakob, Braunschwei, Germany.
 - **Invited** Seminar: An Interdisciplinary Perspective on Predictive Multi-scale Modelling and the Chemisorption of Glycine on Cu(110).
 - March 2016 ISINA Interdisziplinäres Forum, University of Chemnitz, Chemnitz, Germany, Invited talk.
 - March 2016 Prof. Nicholas Zabaras, Engineering Department, Warwick Centre for Predictive Modelling, Warwick, United Kingdom, Invited Seminar.
 - January 2016 Surface Forum Cambridge, Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom.
 - Invited talk: Kinetics of Molecular Diffusion and Self-Assembly: Glycine on Cu {110}
- September 2015 10th European Conference on Computational Chemistry, Fulda, Germany.

 Contributed Talk: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.

- July 2015 Prof. Beate Paulus, Institute of Chemistry and Biochemistry, Freie Universität Berlin, Germany.
 - **Invited** Seminar: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- July 2015 Prof. Bernd Engels, Department of Medicine and Pharmacy, University of Würzburg, Germany.
 - **Invited** Seminar: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- June 2015 Surface Forum Cambridge, BP Institute, University of Cambridge, United Kingdom.

 Invited Talk: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- June 2015 Dassault Systèmes BIOVIA, Science Park, Cambridge, United Kingdom.

 Invited Seminar: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- June 2015 Prof. Patrick Norman, Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden.

 Invited Seminar: Density Embedding Methods: Quality Control and Efficiency for
 - **Invited** Seminar: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- January 2015 A Voyage From Molecules to Materials with Numerical Methods for Quantum Chemistry, Hurtigruten, Norway.

 Invited Talk: Density Embedding Methods: Quality Control and Efficiency for Large
 - **Invited** Talk: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
 - May 2015 Theoretical Chemistry Informal Seminars Series, Department of Chemistry, University of Cambridge, United Kingdom.

 Invited Seminar: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- January 2015 A Voyage From Molecules to Materials with Numerical Methods for Quantum Chemistry, Hurtigruten, Norway.

 Invited Talk: Density Embedding Methods: Quality Control and Efficiency for Large Metal Clusters.
- September 2014 50th Symposium on Theoretical Chemistry, Vienna, Austria.

 Contributed Talk: Chemisorption on Metal Surfaces: The Role of Quantum Tunnelling.
- September 2014 Profs. Marialore Sulpizi and Friederike Schmid, Condensed Matter Theory Group, University of Mainz, Germany.
 - **Invited** Seminar: Chemisorption on Metal Surfaces: The Role of Quantum Tunnelling.
 - August 2014 European Conference on the Dynamics of Molecular Systems, Gothenburg, Sweden.

 Contributed Talk: Chemisorption on Metal Surfaces: The Role of Quantum Tunnelling.
 - August 2014 Energy Landscapes: From Single Molecules to Soft Matter, Durham, United Kingdom.

 Contributed Talk: Chemisorption on Metal Surfaces: The Role of Quantum Tunnelling.
 - July 2014 10th AIMS (American Institute of Mathematical Sciences) Conference on Dynamical Systems, Differential Equations and Applications, Madrid, Spain.

 Invited Talk: Differentiable Manifolds and Feynman's Path Integrals: Efficient Ways to Investigate the Role of Quantum Tunnelling in Chemical Systems.

- June 2014 FEM-EX Oslo Promoting Female Excellence in Theoretical and Computational Chemistry II, Olso, Norway.
 - **Contributed** Talk: Embedding Methods: Improvements, Extensions, and Chemisorption of Methane on Ni(100).
- November 2013 Prof. Adrian Mulholland, Centre for Computational Chemistry, University of Bristol, Bristol, United Kingdom.
 - **Invited** Seminar: Quantum Rates in the Enzyme Glutamate Mutase: the Instanton Method Applied to Large Systems.
- September 2012 Entanglement Based Approaches in Quantum Chemistry, Dresden, Germany.

 Contributed Talk: Improvements to the Instanton Method: Tunnelling in Glutamate Mutase.
 - July 2012 Prof. Lincoln Car, Heidelberg Center for Quantum Dynamics special colloquium, Department of Physics, University of Heidelberg, Heidelberg, Germany.

 Invited Seminar: Improvements to the Instanton Method: Tunnelling in the Enzyme Glutamate Mutase.
 - March 2012 Meeting of the German Physical Society (DPG), Stuttgart, Germany.

 Contributed Talk: Improvements to the Instanton Method: Tunnelling in Large Systems.
- September 2011 Workshop in Philosophy and History of Science, Stuttgart, Germany.

 Invited Talk: The Reaction Mechanism of the Enzyme Glutamate Mutase:

 Experimental and Computational Studies Hand in Hand.
 - March 2011 Prof. Dan Major's group seminar, Department of Chemistry, Bar-Ilan University, Ramat Gan, Israel.

 Invited Seminar: The Radical Reaction in Glutamate Mutase and Quantum Rates for Large Systems.
 - January 2011 Prof. Neil Marsh's group seminar, Department of Chemistry , University of Michigan, Ann Arbor, Michigan, USA.
 - **Invited** Seminar: The Enzyme Glutamate Mutase: Computational Investigations.
- November 2010 Prof. Jens Nørskov's SUNCAT group seminar, SLAC National Accelerator Laboratory, Stanford, California, USA.
 - **Invited** Seminar: Tunnelling Rates in the Enzyme Glutamate Mutase: the Instanton Method Applied to Large Systems.
- November 2010 Prof. Todd Martinez's group seminar, Department of Chemistry, University of Stanford, California, USA.
 - **Invited** Seminar: Tunnelling Rates in the Enzyme Glutamate Mutase: the Instanton Method Applied to Large Systems.
- September 2010 46th Symposium on Theoretical Chemistry, Münster, Germany.

 Contributed talk: Tunnelling Rates in the Enzyme Glutamate Mutase: the Instanton Method Applied to Large Systems.