

Aoife FOGARTY

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CURRENT POSITION

Postdoctoral fellow, Polymer Theory Group of Prof. Dr. Kurt Kremer, Max-Planck-Institut für Polymerforschung, Mainz, Germany (December 2013 – present)

EDUCATION

Doctorat de l'Université Paris 6, France (PhD in Theoretical Physical Chemistry)
September 2013
Mention: Très honorable

Master of Chemistry, University of Edinburgh, UK
May 2010
Degree classification: First
Overall grade: 86/100
Class ranking: 1st

Irish Leaving Certificate (state school-leaving examinations), Republic of Ireland
June 2006
8 A1 grades (maximum grade) at Higher Level
Ranking: joint 2nd of 54100 candidates

PREVIOUS RESEARCH EXPERIENCE

PhD and postdoctoral fellow in Theoretical Physical Chemistry, Ecole Normale Supérieure, Paris, France (October 2010 – November 2013)
PhD adviser: Dr Damien Laage
Thesis title: '*Theoretical study of biomolecular hydration shells: dynamics and influence on biological function*'

'*Deconvolution and distribution analysis of fluorescence decay data from fluorescent analogues of DNA bases*' - Code development for the analysis of experimental data
University of Edinburgh, UK, September 2009 – June 2010
Supervisors: Dr Anita Jones and Dr Philip Camp
Master of Chemistry dissertation research project and vacation research project

'*Temperature transferability of coarse-grained potentials*' - Atomistic molecular dynamics and development of coarse-grained potentials
TU Darmstadt, Germany, May – July 2009
Supervisors: Prof. Dr. Florian Müller-Plathe and Karim Farah

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Vacation research project with Undergraduate Stipendium from the Deutsche Akademische Austauschdienst

'Structures of a binary two-dimensional mixture in an external magnetic field' -

Monte Carlo simulations of a binary colloidal ferrofluid

University of Edinburgh, UK, June – August 2008

Supervisor: Dr Philip Camp

Vacation research project with Undergraduate Research Bursary from the Engineering and Physical Sciences Research Council

TEACHING

- Lectures, tutorials and lab classes, Experimental Chemistry, 1st year undergraduate, Université Pierre et Marie Curie, 2011-2012 and 2012-2013
- Tutorials, Chemical Reactivity, 3rd year undergraduate, Ecole Normale Supérieure, 2010-2011 and 2011-2012

PUBLICATIONS

- K. Farah, A.C. Fogarty, M.C. Böhm and F. Müller-Plathe, 'Temperature dependence of coarse-grained potentials for liquid hexane', *Phys. Chem. Chem. Phys.*, 2011, 13, 2894-2902
- A.C. Fogarty, A.C. Jones and P.J. Camp, 'Extraction of lifetime distributions from fluorescence decays with application to DNA-base analogues', *Phys. Chem. Chem. Phys.*, 2011, 13, 3819-3830
- A.C. Fogarty, E. Duboué-Dijon, F. Sterpone, J.T. Hynes and D. Laage, 'Biomolecular hydration dynamics: a jump model perspective', *Chem. Soc. Rev.*, 2013, 42, 5672-5683
- A.C. Fogarty, F-X. Coudert, A. Boutin and D. Laage, 'Reorientational dynamics of water confined in zeolites', *ChemPhysChem*, 2014, 15, 521-529
- A.C. Fogarty and D. Laage, 'Water dynamics in protein hydration shells: the molecular origin of the dynamical perturbation', *J. Phys. Chem. B*, 2014, 10.1021/jp409805p
- E. Duboué-Dijon, A.C. Fogarty and D. Laage, 'Temperature dependence of hydrophobic hydration dynamics : from retardation to acceleration', *J. Phys. Chem. B*, 2014, 118, 1574–1583

SCIENTIFIC COMMUNICATION

Talks

- 'Biomolecular hydration shell dynamics', Bunsentagung, Karlsruhe, Germany, May 2013
- 'Biomolecular hydration shell dynamics', Journées de Modélisation, Paris, France, May 2013
- 'Enzyme catalysis in organic solvents: the environment contribution', Journées Francophones des Jeunes Physico-Chimistes, Dinard, France, October 2012
- 'An enzymatic reaction in organic solvent', Journée des Jeunes Chercheurs, Ecole Normale Supérieure Paris, France, May 2011

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- 'Structures of a binary two-dimensional mixture in an external magnetic field', Universitas 21 undergraduate research conference, Glasgow, UK, October 2009

Posters

- 'Enzyme catalysis in organic solvents: the environment contribution', Rencontre des Chimistes Théoriciens Francophones, Marseille, France, July 2012
- 'Enzyme catalysis in organic solvents: the environment contribution', Bunsentagung, Leipzig, Germany, May 2012
- 'An enzymatic reaction characterised by QM/MM methods', WATOC, Santiago de Compostella, Spain, July 2011