Dr Theo Keane

EPSRC Doctoral Prize Fellow, Sheffield **MUST Theory Fellow, Newcastle**

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Key Research Interests

- Photochemistry
- Non-adiabatic effects
- Theoretical and computational chemistry
- Relativistic effects

MUST Theory Fellowship, Newcastle University (April 2018 – Present)
Postdoctoral fellowship in the group of Dr Tom Penfold, Newcastle, in collaboration with Prof. Majed Chergui, EPFL. Investigating photodisocciation dynamics of myoglobin, through simulation of fs time-resolved X-ray emission spectroscopy and comparison to experiments.

EPSRC Doctoral Prize Fellowship, University of Sheffield (January 2017 – Present)
Independent postdoctoral fellowship. Investigating mechanism of controllable electron transfer in transition metal complexes using quantum wavepacket dynamics simulations, working with Dr Anthony J.H.M. Meijer and Prof. Julia A. Weinstein and in collaboration with Prof. Graham Worth, UCL.

PhD Chemistry, University of Sheffield (September 2013 – November 2016)
Title: Non-adiabatic effects in transition metal complexes
Supervisors: Dr Anthony J.H.M. Meijer & Prof. Julia A. Weinstein
Investigation of transition metal complexes displaying excited state electron transfer that can be manipulated *via* selective vibrational excitation. Awarded "Turner Prize" for best PhD thesis.

MChem Chemistry, University of Sheffield (September 2009 – June 2013)
1st Class with Honours. 4th year project investigating organometallic catalysis with DFT.

Emanuel School, London (September 2000 – June 2008)
A levels: Chemistry, Maths, Computing; AS level: Physics; 10 GCSEs.

Quantum chemistry

- Detailed knowledge of ground and excited state electronic structure methods, particularly Density Functional Theory and Time-Dependent DFT, including relativistic formalisms.
- Thorough understanding of underlying theoretical basis for excited state molecular processes, specific knowledge of ultrafast spectroscopic techniques.
- Significant experience using a variety of electronic structure packages, including Gaussian, Q-Chem, Turbomole, ORCA and ADF, and the Quantics wavepacket dynamics package.

Teaching and supervision

- PI of two undergraduate research projects (Summer 2015 & 2016, details below). Required teaching of basic quantum chemistry, use of software and Linux, and technical writing. 2016 project resulted in co-authorship for student (publication 6).

- Directly supervised 9 masters students, providing day-to-day assistance and instruction.
- Undergraduate tutorials for 2nd year students (academic year 2015-2016), requiring knowledge of wide range of physical chemistry topics and ability to communicate ideas in an appropriate manner.
- Supervised 3rd year literature review (academic year 2016-2017) of ultrafast spectroscopy, demonstrating broad knowledge of photochemistry.
- In-lab instructor for undergraduate physical chemistry labs. Marked lab scripts, including formal, manuscript-like lab reports.

Leadership and public engagement

- Devised and implemented a departmental scheme, to engage undergraduates with research through summaries of contemporary publications written by PhDs/Postdocs.
- Obtained seed funding for and developed public engagement activity based on light-activated swimming crystals with colleague (poster 8). Demonstrated to >2000 school children.
- Organised & chaired monthly research cluster meetings and seminars, committee member of departmental researchers society.

Professional skills and communication

- Extensive experience collaborating with chemists: on extended research projects (1, 3, 5, 8, 9), with departmental colleagues (2, 6) and through international collaborations (4, 7).
- Experience collaborating with physicists and engineers (published abstract 2), requiring strong communication with individuals with differing domain knowledge and specialities, as well as planning, conflict resolution and management skills.
- Data processing, interpretation, visualization and communication.
- Ability to program in Python. Proficient in the use of technical software (Gnuplot, Octave) and in the use of Linux. See `www.github.com/theochemtheo` for examples.
- Strong technical writing skills and ability to create both long- and short-form documents in LaTeX, Microsoft Word.

Publications († indicates first author of theoretical contribution)

9 *"Directly Coupled vs. Spectator Linkers of Diimine Pt(II) Acetylides –Change the Structure, Keep the Function?"* S.A. Archer, T. Keane†, M. Delor, E. Bevon, A.J. Auty, D. Chekulaev, I.V. Sazanovich, M. Towrie, A.J.H.M. Meijer, J.A. Weinstein, *Chem. Eur. J.*, **2017**, *23*, 18239-18251.

8 *"Directing the Path of Light-Induced Electron Transfer at a Molecular Fork Using Vibrational Excitation"* M. Delor, S.A. Archer, T. Keane†, A.J.H.M. Meijer, I.V. Sazanovich, G.M. Greetham, M.J. Towrie, J.A. Weinstein, *Nature Chem.*, **2017**, *9*, 1099-1104.

7 *"Identifying Electron Transfer Coordinates in Donor-Bridge-Acceptor Systems Using Mode Projection Analysis"* X. Yang, T. Keane, M. Delor, A.J.H.M. Meijer, J.A. Weinstein, E.R. Bittner, *Nature Commun.*, **2017**, *8*, 14554.

6 *"Manganese Tricarbonyl Complexes with Asymmetric 2-Iminopyridine Ligands: Toward Decoupling Steric and Electronic Factors in Electrocatalytic CO_2 Reduction"* S.J.P. Spall, T. Keane†, J. Tory, D.C. Cocker, H. Adams, H. Fowler, A.J.H.M. Meijer, F. Hartl, J.A. Weinstein, *Inorg. Chem.*, **2016**, *55*, 12568-12582.

5 *"^{13}C or not ^{13}C: Selective Synthesis of Asymmetric Carbon-13 Labelled Platinum (II) cis-Acetylides"* S.A. Archer, T. Keane†, M. Delor, A.J.H.M. Meijer, J.A. Weinstein, *Inorg. Chem.*, **2016**, *55*, 8251-8253.

4 *"A Strategy toward the Biomimetic Synthesis of (±)-Morusalbanol A Pentamethyl Ether"* J.T. Tee, T. Keane†, A.J.H.M. Meijer, H. Khaledi, N.A. Rahman, C.F. Chee, *Synthesis*, **2016**, *48*, 2263-2270.

3 *"On the Mechanism of Vibrational Control of Light-Induced Charge Transfer in Donor-Bridge-Acceptor Assemblies"* M. Delor, T. Keane†, P.A. Scattergood, I.V. Sazanovich, G.M. Greetham, M.J. Towrie, A.J.H.M. Meijer, J.A. Weinstein, *Nature Chem.*, **2015**, *7*, 689-695. *(Front cover)*

2 *"Homoleptic Low-Valent Polyazides of Group 14 Elements"* B. Peerless, T. Keane†, A.J.H.M. Meijer, P. Portius, *Chem. Commun.*, **2015**, *51*, 7435-7438. *(Inside front cover)*

1 *"Dynamics of Ground and Excited State Vibrational Relaxation and Energy Transfer in Transition Metal Carbonyls"* M. Delor, I.V. Sazanovich, M. Towrie, S.J.P. Spall, T. Keane†, A.J. Blake, C. Wilson, A.J.H.M. Meijer, J.A. Weinstein, *J. Phys. Chem. B*, **2014**, *118*, 11781-11791.

In Preparation

- *"Dynamics of high-mobility heteroacene compounds"* O. Koryschenska, J. Garrido-Velasco, A. Musser, C. Gidney, A. Auty, T. Keane, A. Stradosmka-Szymczak, A. Iraqi, J. Clark.
- *"Synthesis, chracterization and properties of Ru and Os dyes that absorb across the entire visible region"* E. Baranoff, T. Keane, B.F.E. Curchod.

Grants

5 CoI: *"Steering Electrons along Multiple Pathways by Mode-specific Vibrational Excitation"*, Direct Access grant to Central Laser Facility 1 week
Investigations of directional "vibrational control". Resulted in publication 8. Compounds proposed as a result of grants 1 & 2 also investigated.

4 PI: Royal Society of Chemistry Undergraduate Research Bursary, 2016. £1600
Funding to provide a stipend for an undergraduate student, modelling the mechanism of CO_2 reduction in Mn-based catalysts. Student credited as co-author on publication 6.

3 CoI: Computing resources at the NSCCS 100,000 CPU hours
"Theoretical investigations into non-adiabatic effects in light-harvesting compounds with controllable electron-transfer dynamics". Awarded maximum time quota.

2 PI: EPSRC Vacation Bursary, 2015. £1760
Funding to provide a stipend for an undergraduate student, investigating properties of candidate complexes expected to undergo "vibrational control". One complex identified and as a result synthesised by collaborators, studied at Central Laser Facility (grant 5) and shows predicted behaviour. Publication in preparation.

1 PI: Royal Society of Chemistry Undergraduate Research Bursary, 2015. £1600
Same project as above.

Talks

6 *"Ultrafast Control of Electron Transfer"* Lord Porter Laser Lab Opening, Sheffield, 14/03/2018.

6 *"Controlling Electron Transfer: Insight from Non-Adiabatic Calculations"* Spectroscopy & Dynamics Group, Bristol, 09/02/2018.

5 *"Ultrafast Vibrational Control of Electron Transfer in the Excited State"* LSF and Artemis User Meeting, Oxford, 06/09/2017.

4 *"Understanding Controllable Electron Transfer in Transition Metal Complexes"* Midlands Computational Chemistry Meeting, Sheffield, 26/07/2017.

3 *"Controlling Electron Transfer in the Excited State via Selective Vibrational Excitation"* International Symposium on Photochemistry and Photophysics of Coordination Compounds, XXII, Oxford, 11/07/2017.

2 *"Directional Control of Electron Transfer in Pt(II) Metal Complexes"* Annual Northern Universities Meeting on Chemical Physics, XXVI, Newcastle, 26/07/2016.

1 *"Modulation of Light-Induced Electron Transfer Pathways by Infrared Light Stimulation of Intramolecular Vibrations"* Spectroscopy & Dynamics Group, Bristol, 22/05/2015.

Published Abstracts & Contributions

3 *"Vibrational and Condensed Phase Dynamics: General Discussion"* A. Orr-Ewing, O. Kornilov, T.I. Sølling, T. Keane, M.P. Minitti, H.J. Wörner, O. Schalk, G.M. Roberts, R.S. Minns, C.J. Milne, L. Miseikis, T.J. Penfold, R.J.D. Miller, W, Domcke, M. Centurion, K. Ueda, P.M. Weber, O. Gessner, D.M. Neumark, A. Stolow, J. Yano, S. Mukamel, V.G. Stavros, *Faraday Disc.*, **2016**, *194*, 747-775.

2 *"Construction of a Reduced Chemical Kinetic Mechanism for Petroleum Diesel Autoxidation"* E. Alborzi, S. Blakey, T. Keane†, A.J.H.M. Meijer, *Proc. IASH 2015, 14th International Symposium on Stability, Handling and Use of Liquid Fuels.*, **2015**.

1 *"Controlling Electron Transfer in Condensed Phase with Bond-Specific Infrared Excitation"* M. Delor, P.A. Scattergood, I.V. Sazanovich, T. Keane†, G.M. Greetham, M.J. Towrie, A.W. Parker, A.J.H.M. Meijer, J.A. Weinstein, *Proc. SPIE 9549, Physical Chemistry of Interfaces and Nanomaterials XIV*, **2015**, 959490U.

Posters

9 *"Dynamics of Vibrationally Controllable Electron Transfer"*, T. Keane, A.J.H.M Meijer, J.A. Weinstein, *Electron Donor-Acceptor Interactions GRC*, Newport RI, *scheduled* August 2018.

8 *"The Molecular Boat Race"*, T. Keane, T. Roseveare, J.S. Wright, *IUPAC International Conference on Chemical Education XV*, Sydney, *scheduled* July 2018.

7 *"Controlling Electron Transfer Through Selective Vibrational Excitation"*, T. Keane, M. Delor, J.A. Weinstein, A.J.H.M. Meijer, *WATOC XI*, Munich, 2017.

6 *"Directionally Controllable Electron Transfer in a Chemically Symmetrical D-B-A-B-D Pentad"*, T. Keane, M. Delor, S.A. Archer, J.A. Weinstein, A.J.H.M. Meijer, *Faraday Discussion: Ultrafast Imaging of Photochemical Dynamics*, Edinburgh, 2016.

5 *"Computational Investigations into Light Induced Control of Electron Transfer"*, T. Keane, M. Delor, J.A. Weinstein, A.J.H.M. Meijer, *RSC Spectroscopy and Dynamics Group Meeting*, Warwick, 2016.

4 *"Computational Investigations into Light Induced Control of Electron Transfer"*, T. Keane, M. Delor, J.A. Weinstein, A.J.H.M. Meijer, *Annual Northern Universities Meeting on Chemical Physics XXV*, Leeds, 2015.

3 *"Computational Investigations into Light Induced Control of Electron Transfer"*, T. Keane, M. Delor, J.A. Weinstein, A.J.H.M. Meijer, *Modelling Photoactive Molecules 2015*, Nantes, 2015.

2 *"Predicting the Properties of Pt(II) Donor-Acceptor Complexes Using Density Functional Theory (DFT)"*, T. Keane, S. Archer, J.A. Weinstein, A.J.H.M. Meijer, *UKTC2014*, Oxford, 2014.

1 *"Rate Enhancement in the S_N2 Reaction Between CH_3I and $[Rh(CO)(I)(PN^{oAn})]$"*, T. Keane, A.J.H.M. Meijer, *HPC@Sheffield2014*, Sheffield, 2014.

Professional Membership & Service

Member RSC; Member ACS; Lifetime Member WATOC. Grant reviewer RSC 2017-2018.