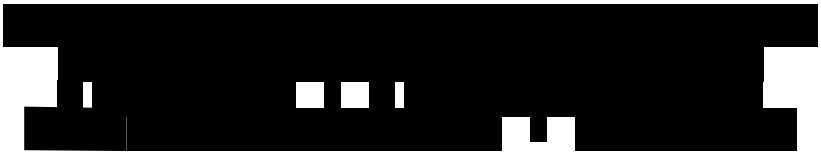
James Alexander Green | Curriculum Vitae



Research Interests

- : Theoretical/computational chemistry for photochemistry of technologically and biologically relevant molecules.
- : Nonadiabatic quantum dynamics, including both trajectory and wavepacket approaches.
- : Excitonic modelling of multichromophoric systems.
- : Development and application of electronic structure theory methods, in particular density functional theory.

Research Experience

Goethe University **Frankfurt am Main, Germany**
Alexander von Humboldt Postdoctoral Fellow, Supervisor: Prof. Irene Burghardt *01/06/2022–present*
Theoretical modelling of organic semiconductor and photovoltaic materials, and computation of their multidimensional time-resolved spectroscopies using quantum dynamics and electronic structure theory.

Italian National Research Council **Naples, Italy**
Postdoctoral Research Assistant, Supervisor: Dr. Roberto Improta *14/03/2019–13/03/2022*
Theoretical modelling of the excited states and spectroscopy of DNA, on a variety of scales with a variety of methods. Quantum wavepacket dynamics of the single nucleobases, base pairs, and double helix, including calculation of absorption spectra and solvent effect. Simulation of the electronic circular dichroism spectra of guanine quadruplexes via development of an excitonic model incorporating charge transfer states. Development of a diabatisation strategy and open-source program code, *Overdia*, to parameterise model Hamiltonians for single and multi-chromophore systems.

University of Leeds **Leeds, United Kingdom**
Postdoctoral Research Assistant, Supervisor: Prof. Dmitry Shalashilin *01/04/2018–31/12/2018*
Theoretical support to a joint theoretical and experimental investigation in collaboration with the group of Prof. Vasilios Stavros at the University of Warwick on the ultrafast photodissociation of 2-ethylpyrrole, pyrazole, and imidazole. Lead theoretical researcher studying 2-ethylpyrrole, investigating the photodissociation using trajectory guided quantum dynamics. Provided electronic structure support to the pyrazole and imidazole investigations.

University of Manchester **Manchester, United Kingdom**
Nuffield Summer Project, Supervisor: Dr. Richard Henchman *03/07/2009–07/08/2009*
5-week summer project involving a molecular dynamics investigation of Troutons and Hildebrands rules for the entropy of vaporization of a liquid. A molecular interpretation for the entropy was obtained, being able to be calculated from the forces obtained from molecular dynamics calculations of various liquids.

Education

University of Leeds **Leeds, United Kingdom**
PhD, Supervisor: Prof. Dmitry Shalashilin *01/10/2014–30/04/2018*
Thesis entitled: "Development and Application of New Numerical Extensions to the Coupled Coherent States Family of Multidimensional Quantum Dynamics Methods", and the project involved the development of two new numerical extensions. The first, a two-layer version of the coupled coherent states method permitted additional flexibility in the wavefunction representation, as well as improved numerical efficiency and parallel scalability.

The second permitted the coupled coherent states method to study systems of indistinguishable bosons, such as Bose-Einstein condensates. Both extensions were applied to a model tunnelling problem, which I also produced a benchmark calculation for.

Durham University **Durham, United Kingdom**

MChem, 1st Class Hons., Masters project supervisor: Prof. David Tozer *04/10/2010–02/07/2014*

Four year integrated bachelors and masters program. 1st class marks in all lecture courses, including: organic, inorganic and physical chemistry; computational chemistry; materials chemistry; and mathematics. Final year Masters project with Prof. David Tozer entitled "Non-interacting Kinetic Energy Functionals in Density Functional Theory." Orbital-free functionals were developed, with a focus on correctly predicting molecular binding for a test series of molecules, which previous orbital-free non-interacting kinetic energy functionals failed to do.

Publications

1.: A. Segalina, D. Aranda, J. A. Green, V. Cristino, S. Caramori, G. Prampolini, M. Pastore, and F. Santoro, "How the Interplay among Conformational Disorder, Solvation, Local, and Charge-Transfer Excitations Affects the Absorption Spectrum and Photoinduced Dynamics of Perylene Diimide Dimers: A Molecular Dynamics/Quantum Vibronic Approach.", *J. Chem. Theory. Comput.*, Accepted.

2.: M. Yaghoubi Jouybari, J. A. Green, R. Improta, & F. Santoro, "The ultrafast quantum dynamics of photoexcited adenine-thymine basepair investigated with a fragment-based diabatisation and a linear vibronic coupling model.", *J. Phys. Chem. A*, 2021, **125**, 8912.

3.: H. Asha, J. A. Green, L. Martinez-Fernandez, L. Esposito, & R. Improta, "Electronic circular dichroism spectra of DNA quadruple helices studied by molecular dynamics simulations and excitonic calculations including charge transfer states", *Molecules*, 2021, **26**, 4789.

4.: J. A. Green, M. Yaghoubi Jouybari, H. Asha, F. Santoro, & R. Improta, "Fragment diabatization linear vibronic coupling model for quantum dynamics of multichromophoric systems: population of the charge-transfer state in the photoexcited guanine–cytosine pair", *J. Chem. Theory. Comput.*, 2021, **17**, 4660.

5.: F. Santoro, J. A. Green, L. Martinez-Fernandez, J. Cerezo, & R. Improta, "Quantum and semiclassical dynamical studies of nonadiabatic processes in solution: achievements and perspectives", *Phys. Chem. Chem. Phys.*, 2021, **23**, 8181.

6.: J. A. Green, M. Yaghoubi Jouybari, D. Aranda, R. Improta, & F. Santoro, "Nonadiabatic absorption spectra and ultrafast dynamics of DNA and RNA photoexcited nucleobases", *Molecules*, 2021, **26**, 1743.

7.: J. A. Green, H. Asha, F. Santoro, & R. Improta "Excitonic model for strongly coupled multichromophoric systems: the electronic circular dichroism spectra of guanine quadruplexes as test cases", *J. Chem. Theory. Comput.*, 2021, **17**, 405.

8.: J. A. Green & R. Improta, "Vibrations of the guanine–cytosine pair in chloroform: an anharmonic computational study", *Phys. Chem. Chem. Phys.*, 2020, **22**, 5509.

9.: J. A. Green & D. V. Shalashilin, "Simulation of the quantum dynamics of indistinguishable bosons with the method of coupled coherent states", *Phys. Rev. A*, 2019, **100**, 013607.

10.: C. Symonds, D. V. Makhov, N. C. Cole-Filipiak, J. A. Green, V. G. Stavros, & D. V. Shalashilin, "Ultrafast photodissociation dynamics of pyrazole, imidazole and their deuterated derivatives using *ab initio* multiple cloning", *Phys. Chem. Chem. Phys.*, 2019, **21**, 9987.

11.: J. A. Green, D. V. Makhov, N. C. Cole-Filipiak, C. Symonds, V. G. Stavros, & D. V. Shalashilin, "Ultrafast photodissociation dynamics of 2-ethylpyrrole: adding insight to experiment with *ab initio* multiple cloning", *Phys.*

Chem. Chem. Phys., 2019, **21**, 3832.

12.: J. A. Green, A. Grigolo, M. Ronto, & D. V. Shalashilin, "A two-layer approach to the coupled coherent states method", *J. Chem. Phys.*, 2016, **144**, 024111.

13.: J. A. Green & D. V. Shalashilin, "Benchmark calculation for tunnelling through a multidimensional asymmetric double well potential", *Chem. Phys. Lett.*, 2015, **641**, 173.

14.: A. Borgoo, J. A. Green, & D. J. Tozer, "Molecular binding in post-Kohn–Sham orbital-free DFT", *J. Chem. Theory Comput.*, 2014, **10**, 5338.

15.: J. A. Green, S. J. Irudayam, & R. H. Henchman, "Molecular interpretation of Trouton's and Hildebrand's rules for the entropy of vaporization of a liquid", *J. Chem. Therm.*, 2011, **43**, 868

Presentations

Invited Talks

02/02/2022: Institute of Chemical Sciences Seminar, Heriot-Watt University (Online - Edinburgh, UK)

15/05/2019: Chemistry Seminar, CNR-ICCOM (Pisa, Italy)

11/07/2016: Theoretical Chemistry Seminar, Heidelberg University (Heidelberg, Germany)

Contributed Talks

20/09/2021: 57th Symposium on Theoretical Chemistry, Universität Würzburg (Online)

20/01/2021: CπC Virtual (Online)

11/01/2021: RSC Spectroscopy & Dynamics Workshop Group Meeting 2021 (Online)

06/02/2020: Modelling Photoinduced Processes in Molecular Systems (London, UK)

31/01/2020: CπC 11 (Zagreb, Croatia)

14/12/2018: School of Chemistry Postdoctoral Conference 2018 (Leeds, UK)

10/01/2018: RSC Spectroscopy & Dynamics Workshop Group Meeting 2018 (Durham, UK)

08/06/2017: School of Chemistry Postgraduate Conference 2017 (Leeds, UK)

Flash Talks

16/06/2021: Principles of Light-induced Charge Transfer for Optogenetics Workshop (Online)

04/05/2021: Les Houches Workshop: Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems (Online)

Poster Presentations

28/11/2018: Workshop on Atomic Physics 2018: Trajectories in AMOP Physics (Dresden, Germany)

04/09/2018: 10th International Meeting on Photodynamics and Related Aspects (Cartagena, Colombia)

20/03/2017: Computational Molecular Science 2017 (Warwick, UK)

02/09/2016: 5th International Workshop on High Dimensional Quantum Dynamics (Rostock, Germany)

09/06/2016: School of Chemistry Postgraduate Conference 2016 (Leeds, UK)

16/03/2015: Computational Molecular Science 2015 (Warwick, UK)

Tutorial Lectures

18/02/2020: LightDyNAmics Technology Training Camp (Vienna, Austria)

Software Development

▪ : *Overdia*: Co-author of this free open source program code with F. Santoro aimed at the definition of diabatic electronic states and the parametrization of model Hamiltonians from Time-Dependent Density Functional Theory calculations. `http://www.iccom.cnr.it/en/overdia-en/`

Teaching Experience

Postgraduate Demonstrator University of Leeds **01/10/2014–31/03/2018**

One session per week in the physical chemistry laboratory and one class per week in the "maths for chemists" workshop.

Management and Leadership Activities

LightDyNAmics Marie Sklodowska-Curie European Training Network **14/03/2019–13/03/2022**

Assisting the coordinator of the network, Dr. Roberto Improta, with organising training meetings, webinars, preparation of deliverables to submit to the European Commission, and co-ordination of the 15 Early Stage Researchers (ESRs) and 14 Principal Investigators (PIs) at 13 EU institutes involved in the network.

Postgraduate Representative for University of Leeds Chemistry **01/01/2017–01/10/2017**

Collected views, questions and issues raised by PhD students in the department and presented them to faculty, graduate school, and university committees to provide support and affect policy change.

Industrial Advisory Board Liason for University of Leeds Postgraduate Chemists01/06/2016–31/12/2016

Provided support to PhD students seeking industrial employment by bringing forward questions to the industrial advisory board affiliated with the University of Leeds chemistry department about where they could search for jobs, and fed back relevant contacts.

President of the University of Leeds Postgraduate Chemistry Committee **01/07/2015–01/10/2016**

Organised social events for postgraduate students and staff within the chemistry department. Invited a keynote speaker and secured sponsorship for the end of year postgraduate chemistry conference.

Workshop, Seminar, and Conference Organisation

LightDyNAmics Research Webinars **23/04/2020–15/11/2021**
Organiser *Online*

Mixture of research presentations, journal club, and tutorial seminars given by the LightDyNAmics ESRs. Sessions conducted on conducted on 23/04/20, 22/07/20, 25/02/21, 12/07/21 and 15/11/21.

3rd LightDyNAmics Week Pt. 2 **15/11/2021–17/11/2021**
Co-organiser *Université Paris-Saclay*

'Day of Light and Matter' talks by invited speakers, management board meeting, and led workshop sessions for the ESRs.

3rd LightDyNAmics Week Pt. 1 **12/07/2021–14/07/2021**
Co-organiser *Online*

Research presentations by ESRs (chair for all talks), management board meeting, proposal writing session, and led a careers session.

2nd LightDyNAmics Week Pt. 2 **30/04/2021**
Co-organiser *Online*

Photosynthesis lecture by Dr. Bruno Robert and outreach experiment design by Dr. Jonathan Piard.

Molecular Horizon and Molecular Discovery Workshop **14/12/2020–18/12/2020**
Co-organiser *Online*

Overview of working in industry for the ESRs in the LightDyNAmics network.

2nd LightDyNAmics Week Pt. 1 **28/10/2020–29/10/2020**
Co-organiser *Online*

Research presentations by ESRs and management board meeting.

LightDyNAmics Technology Training Camp **17/02/2020–21/02/2020**
Co-organiser *University of Vienna*
Tutorial lectures and workshop week on experimental and theoretical methods for photochemistry.

1st LightDyNAmics Week **17/06/2019–21/06/2019**
Co-organiser *University of Bologna*
Research presentations by ESRs and tutorial lectures by PIs.

Outreach Activities

LightDyNAmics Twitter **14/03/2019–13/03/2022**

Management of LightDyNAmics twitter account, publicising results from the network

Discovery Lab 2.0: Ricerca per passione VII edizione **30/09/2020**

Outreach talk to secondary school students: 'Quantum Mechanics Calculations in Real Life'

Bright Club Co-Organiser **01/10/2015–30/04/2016**

Helped re-form the Bright Club academic outreach stand up comedy night in Leeds. Put on 3 events where academics from a variety of disciplines performed a stand up routine on their research, or experiences of it, and personally performed at 2 of the events.

Prizes and Awards

- : **Marie-Curie Seal of Excellence** Awarded to the proposal "Development of a theoretical toolkit to investigate energy transport in multi-chromophore systems with squaraine excitonic dynamics and 2-dimensional electronic spectroscopy", *2022*.
- : **Spectroscopy and Dynamics Group Meeting 2021 2nd Place Best Talk Prize**, *2021*.
- : **CpiC 11 Best Talk Prize**, *2020*.
- : **Lindau Nobel Laureate Conference Young Researcher**, *2017*, selected as University of Leeds representative to attend 67th Lindau Nobel Laureate Conference, Lindau.
- : **University of Leeds Chemistry Postgraduate Conference Best Poster Prize**, *2016*.
- : **Dr. Kate Furneaux Prize**, *2016*, most meritorious non-academic contribution to postgraduate life in the School of Chemistry during the academic year.
- : **CREST Gold Award**, *2009* British Science Association award for conducting original research when aged 16.

Grants and Funding

- : **Alexander von Humboldt Postdoctoral Fellowship** Two years funding awarded for the project "Excited State Processes in Squaraine Dyes Targeted for Organic Photovoltaics".
- : **Royal Society - Italian National Research Council Joint Project**, *2021-2022*, co-author and co-beneficiary of a UK-Italy travel grant on the project "Photoexcited DNA nucleobases: Towards complete quantum dynamics simulations including solvent."
- : **University Research Scholarship**, *2014-2018*, PhD funding awarded by the University of Leeds to a limited number of students on the basis of excellent academic achievement.
- : **Nuffield Research Bursary**, *2009*, funding to carry out a 5-week research placement during summer 2009 with Dr. Richard Henchman at the University of Manchester.

Supervision and Mentoring

- : Co-supervision of two ESRs in the LightDyNAmics project, in the groups of R. Improta and F. Santoro.

Additional Academic Activities

- : Reviewer for *Phys. Chem. Chem. Phys.*, *ChemPhysChem*, and *Biopolymers*.