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## Antonios M. Alvertis

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Nationality: Greek

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### EMPLOYMENT

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**Aug 2023 – Present      Research Scientist – NASA Ames Research Center**

- Developing first-principles approaches for rigorously mapping complex materials problems onto model Hamiltonians amenable to efficient solution on quantum hardware, and accounting for strong electronic correlations and finite-temperature effects on equal footing.

**Apr 2021 – Aug 2023      Winton Exchange Research Fellow & Postdoctoral Researcher – Lawrence Berkeley National Laboratory**  
Supervisor: Prof. Jeffrey Neaton

- Conceived of and published a study that was **featured on the cover of Physical Review Letters** (ref. [4] in publication list below).
- Developed *a theory and efficient computational workflow* to extend first-principles calculations of excited states to account for the effects of temperature (ref. [1]).
- Developed theoretical and computational methods for quantum many-body dynamics in a wide range of solids and molecular systems (refs. [1]-[9]).

### EDUCATION

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**Oct 2017 – Mar 2021      PhD Physics – University of Cambridge**  
“On exciton-vibration and exciton-photon interactions in organic semiconductors”  
Supervisors: Dr Alex Chin and Dr Akshay Rao

- Won the *Springer Ph.D. thesis prize* after my thesis was nominated as the most outstanding doctoral contribution from the Cambridge Physics Department, for 2020-2021. The thesis was published as a part of the “Springer Theses” book series: <https://link.springer.com/book/10.1007/978-3-030-85454-6>.
- Won the annual *Cavendish PhD prize* in Computational Physics.
- Co-authored six publications (references [10]-[15] in publication list). I am corresponding author for three, and the lead theoretician for the remaining three, which are collaborations with experimental groups that I initiated.

**2016 – 2017      MPhil Scientific Computing – University of Cambridge**  
Awarded with distinction (83.4/100)

**2014 – 2016      MSc Organic and Molecular Electronics – TU Dresden**  
Awarded with Distinction, First Class (1.2/1.0)

**2010 – 2014      BSc Physics – National and Kapodistrian University of Athens**  
Awarded with Distinction (9.61/10)

## AWARDS AND HONORS

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2023-2024	<b>NERSC Director's Discretionary Reserve Year 2023 award</b> 4,000 CPU and 4,000 GPU Node Hours award on the NERSC supercomputer, for my proposed project "Quantum Simulation of downfolded material Hamiltonians", on which I am the principal investigator.
2021-2022	<b>Winton Postdoctoral Exchange Research Fellowship</b> £ 44,816 for research and living expenses to undertake a research stay of 12 months at UC Berkeley, awarded by the Winton Programme for the Physics of Sustainability.
April 2021	<b>Springer Ph.D. thesis prize</b> My thesis was nominated by the Cavendish laboratory as the most outstanding doctoral piece of work of my cohort, winning the Springer Ph.D. thesis prize and a €500 monetary award.
2020	<b>Cavendish PhD prize in Computational Physics</b> This annual prize of £500 was awarded to me for the entirety of my PhD research, on the basis of my paper published in <i>Physical Review B</i> [5].
2016-2020	<b>EPSRC Studentship</b> £14,296 per annum covering living expenses during my MPhil and PhD studies at the University of Cambridge. £9,468 per annum for covering tuition fees. £3,700 for conference/travel expenses.
2016-2020	<b>Winton Scholarship</b> £5,000 for conference/travel expenses and Honorary Scholar of the Winton Programme for the Physics of Sustainability.
2020	<b>Santander Award, St Edmund's College</b> £500 award to support a research trip in the US in February of 2020, during which I visited groups at Columbia and Cornell Universities.
2019	<b>Winton – Berkeley Exchange Award</b> \$5,528 in support of a research stay of two months at the group of Prof. Jeffrey Neaton at UC Berkeley, California.
2017	<b>Santander Award, St Edmund's College</b> £500 award for achieving distinction in my MPhil studies and continuing towards a PhD at the University of Cambridge.
2014-2016	<b>German Academic Exchange Service (DAAD) Scholarship</b> €17,500 over 2 years of M.Sc. studies at the TU Dresden.
2015	<b>Novald excellence scholarship</b> €1,800 awarded from the company Novald for being the first of my class during my M.Sc. studies at the TU Dresden.
2010-2014	<b>Greek State Scholarships Excellence awards</b> €3,740 (combination of four different awards) awarded for achieving excellence in my undergraduate studies.
2010-2014	<b>Antonios Papadakis full undergraduate scholarship</b> €14,400 in support of my undergraduate studies at the National and Kapodistrian University of Athens.

## INVITED TALKS AND PRESENTATIONS

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“First-principles modeling of excited states at finite temperatures: phonon-induced localization, dissociation and screening”, March 2024, **APS March Meeting**

“Phonon-induced screening and dissociation of excitons from first principles”, February 2023, **Berkeley Excited State Conference**

“Theoretical description of exciton-vibration coupling in solid- and gas-phase organic molecules”, March 2022, **Pitzer Center Theoretical Chemistry Seminar, UC Berkeley, USA**

“Impact of strong exciton-phonon interactions and anharmonicity on the optoelectronic properties of organic semiconductors”, December 2021, **CECAM workshop on Exciton Dynamics in Functional Materials**

“Non-perturbative exciton-phonon interactions and anharmonic effects in organic semiconductors”, October 2021, Jornada group, **Stanford University, USA**

“Modelling strong exciton-vibration interactions in organic structures”, April 2021, **Weizmann Institute of Science, Israel** (remote)

“Modelling of ultrafast processes in organic semiconductors using tensor network methods”, February 2020, Reichman group, **Columbia University, USA** & theory journal club, **Cornell University, USA**

“Exciton temperature dependence dictated by localization in organic semiconductors”, June 2019, Neaton group, **UC Berkeley, USA**

“Non-equilibrium relaxation of hot states in organic semiconductors”, June 2019, Chan group, **California Institute of Technology, USA** & June 2019, Yuen Zhou group, **UC San Diego, USA**

“Controlling the coherence of intramolecular singlet fission”, April 2019, **California State University, East Bay, USA** & October 2018, **University of Mons, Belgium**

“Tensor network simulation of ultrafast singlet fission dynamics”, February 2018, Verstraete group, **University of Ghent, Belgium** & January 2018, **IFW Dresden, Germany**

## CONTRIBUTED TALKS/POSTERS AT INTERNATIONAL CONFERENCES

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March 2024	Oral (contributed) presentation at the annual March meeting for the American Physical Society, taking place in Minneapolis.
May 2023	Oral presentation at the “West Coast Theoretical Chemistry Meeting” at UC Davis.
March 2023	Oral presentation at the annual March meeting for the American Physical Society, taking place in Las Vegas.
August 2022	Oral presentation at the Psi-k 2022 conference in EPFL, Lausanne, as a part of the symposium “Polarons and excitons: fundamentals of charge trapping and its impact on applications”.
March 2022	Oral presentation at the annual March meeting for the American Physical Society, taking place in Chicago.
July 2021	Poster presentation at the (on-line) “International Workshop on Recent Developments in Electronic Structure”, organised by the Simons Foundation.

June 2021	Oral presentation at the (on-line) “International Workshop on Charge Transport and Excited State Processes in Organic Materials”, organised by University College London.
March 2021	Oral presentation at the (on-line) annual meeting of the American Physical Society.
November 2020	Oral presentation at the (on-line) annual meeting for the American Materials Research Society.
November 2020	Oral presentation at the (on-line) “International conference on electron-phonon coupling and thermoelectric efficiency”.
September 2020	Poster presentation at the (on-line) “Workshop on the Excited Charge Dynamics in Semiconductors”, organized by the Abdus Salam Centre for Theoretical Physics (ICTP).
February 2020	Poster presentation at the annual meeting of the “Simons Collaboration on Localization of Waves” in New York, at the invitation of Professor Sir Richard Friend (Cavendish).
September 2019	Oral presentation at the “24 <sup>th</sup> European Theoretical Spectroscopy Facility (ETSF) Workshop on Electronic Excitations”, Jena, Germany.
September 2019	Poster presentation at the “Quantum effects in complex systems Faraday Discussions, Coventry, United Kingdom.
May 2019	Poster presentation at the “Simons Wave Collaboration – Short Course & Workshop: Quantum Mechanics and Semiconductors”, Santa Barbara, California, United States.
July 2018	Poster presentation at the Gordon Research conference on “Electronic Processes in Organic Materials”, Barga, Italy.
July 2018	Oral presentation at the Gordon Research Seminar on “Electronic Processes in Organic Materials”, Barga, Italy.
April 2018	Poster presentation at the “2 <sup>nd</sup> International Symposium on Singlet Fission and Photon Fusion: Emerging Solar Energy Technologies”, Gothenburg, Sweden.

## ORGANIZATIONAL EXPERIENCE AND FUNDING

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2023	Co-organizer of the annual BerkeleyGW software package workshop at UC Berkeley, educating graduate researchers on advanced computational techniques for materials science.
2022	Co-organizer and chair of the symposium “Excitons in complex materials” in EPFL, Lausanne, as a part of the 5-year general conference of the Psi-k community: <a href="https://www.psi2022.net">https://www.psi2022.net</a> .
2021-2022	Designed and submitted a successful proposal for £ 44,816 to promote a 12-month collaboration between the University of Cambridge and UC Berkeley, during which I spent six months at each institution.
2021	Contributed to a successful proposal for 40M CPU hours on the NERSC high-performance computing system in the USA.

2021	Co-designed and submitted a successful proposal for 8M CPU hours on the CSD3 high-performance computing system in the UK.
2020	Co-designed and submitted a successful proposal for 6M CPU hours on the CSD3 high-performance computing system in the UK.
2018	Co-organized the annual graduate student conference of the Physics Department of the University of Cambridge.

## TEACHING AND RESEARCH SUPERVISION EXPERIENCE

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February 2023	Tutor of the annual BerkeleyGW software package workshop at UC Berkeley, educating graduate researchers on advanced computational techniques for materials science.
January 2022	Tutored graduate students and researchers on advanced computational modelling methods within the BerkeleyGW software package as a part of the annual BerkeleyGW workshop at UC Berkeley.
2021-2022	Mentored a Ph.D. student at the University of Cambridge for the theory part of a project, in collaboration with the experimental group of Dr. Akshay Rao, resulting in a publication in <i>Nature</i> [3].
2020-2021	Designed and co-supervised a B.Sc. thesis at the National and Kapodistrian University of Athens, as a part of a collaboration with the group of Professor Constantinos Simserides.
2017 – 2021	Supervised third year physics University of Cambridge undergraduate students in Advanced Quantum Physics (more than forty students in total).
2017 – 2018	Supervised second year University of Cambridge undergraduate students in Part IB Physics, which includes classical mechanics, electromagnetism, thermodynamics and statistical mechanics.

## PUBLICATIONS

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[1] **Antonios M. Alvertis**, Jonah B. Haber, Zhenglu Li, Christopher J.N. Coveney, Steven G. Louie, Marina R. Filip, Jeffrey B. Neaton. "Phonon screening and dissociation of excitons at finite temperatures from first principles". *Proceedings of the National Academy of Sciences* 121, e2403434121 (2024)

[2] **Antonios M. Alvertis\***, David Williams-Young, Fabien Bruneval, Jeffrey B. Neaton. "Influence of electronic correlations on electron-phonon interactions of molecular systems with the GW and coupled cluster methods". *Journal of Chemical Theory and Computation* (2024)

[3] Pratyush Ghosh, **Antonios M Alvertis**, Rituparno Chowdhury, Petri Murto, Alexander J Gillett, Shengzhi Dong, Alexander J Sneyd, Hwan-Hee Cho, Emrys W Evans, Bartomeu Monserrat, Feng Li, Christoph Schnedermann, Hugo Bronstein, Richard H Friend, Akshay Rao. "Decoupling excitons from high-frequency vibrations in organic molecules". *Nature*, 629, 355 (2024)

[4] **Antonios M. Alvertis\***, Aurelie Champagne, Mauro Del Ben, Diana Qiu, Felipe H. da Jornada, Marina R. Filip, Jeffrey B. Neaton. "Importance of nonuniform Brillouin zone sampling for *ab initio* Bethe-Salpeter equation calculations of exciton binding energies in crystalline solids". *Physical Review B*, 108, 235117 (2023) (**Editor's Suggestion**)

[5] **Antonios M. Alvertis\***, Jonah B. Haber, Edgar A. Engel, Sahar Sharifzadeh, Jeffrey B. Neaton. "Phonon-induced exciton localization in molecular crystals from first principles". *Physical Review Letters*, 130, 086401 (2023) (**Featured on the cover of the journal**)

[6] Alexander J. Gillett, Anton Pershin, Raj Pandya, Sascha Feldmann, Alexander J. Sneyd, **Antonios M. Alvertis**, Emrys W. Evans, Tudor H. Thomas, Lin-Song Cui, Bluebell H. Drummond, Gregory D. Scholes, Yoann Olivier, Akshay Rao, Richard H. Friend, David Beljonne. "Dielectric control of reverse intersystem crossing in thermally activated delayed fluorescence emitters". *Nature Materials*, 21, 1150 (2022)

[5] **Antonios M. Alvertis\*** and Edgar A. Engel. "Importance of vibrational anharmonicity for electron-phonon coupling in molecular crystals". *Physical Review B*, 105, L180301 (2022)

[7] Konstantinos Lambropoulos, **Antonios M. Alvertis**, Andreas Morphis, Constantinos Simserides "Cyclo[18]carbon including zero-point motion: ground state, first singlet and triplet excitations, and hole transfer". *Physical Chemistry Chemical Physics* 24, 7779 (2022)

[8] Raj Pandya, ..., **Antonios M. Alvertis**, *et al.* "Microcavity-like exciton-polaritons can be the primary photoexcitation in bare organic semiconductors". *Nature Communications*, 12:6519 (2022)

[9] Timothy J. H. Hele, Bartomeu Monserrat, **Antonios M. Alvertis\***. "Systematic improvement of molecular excited state calculations by inclusion of nuclear quantum motion: a mode-resolved picture and the effect of molecular size". *The Journal of Chemical Physics*, 154, 244109 (2021)

[10] Raj Pandya, **Antonios M. Alvertis**, Qifei Gu, Jooyoung Sung, Laurent Legrand, David Kreher, Thierry Barisien, Alex W. Chin, Christoph Schnedermann, Akshay Rao. "Exciton diffusion in highly-ordered one dimensional conjugated polymers: effects of back-bone torsion, electronic symmetry, phonons and annihilation". *The Journal of Physical Chemistry Letters*, 12, 3669 (2021)

[11] **Antonios M. Alvertis\***, Raj Pandya, Loreta A. Muscarella, Nipun Sawhney, Malgorzata Nguyen, Bruno Ehrler, Akshay Rao, Richard H. Friend, Alex W. Chin. Bartomeu Monserrat "Impact of exciton delocalization on exciton-vibration interactions in organic semiconductors". *Physical Review B*, 102, 081122(R) (2020)

[12] **Antonios M. Alvertis\***, Raj Pandya, Claudio Quarti, Laurent Legrand, Thierry Barisien, Bartomeu Monserrat, Andrew J. Musser, Akshay Rao, Alex W. Chin, David Beljonne. "First principles modeling of exciton-polaritons in polydiacetylene chains". *The Journal of Chemical Physics*, 153, 084103 (2020)

[13] **Antonios M. Alvertis**, Steven Lukman, Timothy J. H. Hele, Eric G. Fuemmeler, Jiaqi Feng, Jishan Wu, Neil C. Greenham, Alex W. Chin, Andrew J. Musser. "Switching between coherent and incoherent singlet fission via solvent-induced symmetry-breaking". *Journal of the American Chemical Society*, 141, 44, 17558-17570 (2019)

[14] Christoph Schnedermann, **Antonios M. Alvertis**, Torsten Wende, Steven Lukman, Jiaqi Feng, Florian A.Y.N. Schröder, David H.P. Turban, Jishan Wu, Nicholas D.M. Hine, Neil C. Greenham, Alex W. Chin, Akshay Rao, Philipp Kukura, Andrew J. Musser. "A Molecular Movie of Ultrafast Singlet Fission". *Nature Communications*, 10:4207 (2019)

[15] **Antonios M. Alvertis\***, Florian A.Y.N. Schröder, Alex W. Chin. "Non-equilibrium relaxation of hot states in organic semiconductors: impact of mode-selective excitation on charge transfer". *The Journal of Chemical Physics*, 151, 084104 (2019)

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