PERSONAL INFORMATION

Family name, First name: Zacharias, Marios Date of birth: 12/07/1989
ORCID: 0000-0002-7052-5684, Researcher ID: X 8676 2019

EMPLOYMENT

1 May 2019 – present – Lemesos, Cyprus

Postdoctoral fellow - Cyprus University of Technology

- Projects on computational materials science:
  Temperature dependence of the optical and electronic properties of nanocrystal structures
  Thermal and nonequilibrium diffuse scattering in solids from first-principles
  (with Prof. P. C. Kelires, Research Unit for Nanostructured Materials Systems)
- Computational packages used: *Quantum Espresso, FHI-aims, PHONOPY*
- Supervision of A. Fikardos for the project:
  High-throughput calculations of diffuse scattering in 2D materials via AiiDA

1 October 2018 – 1 January 2020 – Berlin, Germany

Postdoctoral fellow - Fritz-Haber-Institute of the Max Planck Society

- Project on computational materials science:
  Electronic transport in thermoelectric perovskites: systematic consideration of anharmonicity
  (with Dr. C. Carbogno, and Prof. M. Scheffler, Theory Department, NOMAD laboratory)
- Computational packages used: *FHI-aims, PHONOPY*
- Supervision of Z. Yuan for the project:
  Fully anharmonic, first-principles theory of electronic transport

14 August 2017 – 14 August 2018 – Oxford, United Kingdom

Postdoctoral fellow - University of Oxford

- Project on computational materials science:
  Optical properties of materials at finite temperatures for photovoltaic applications
  (with Prof. F. Giustino, Materials Modelling Laboratory)
- Computational packages used: *Quantum Espresso, EPW, YAMBO*

EDUCATION

14 October 2013 – 12 December 2017 – Oxford, United Kingdom

Ph.D. in Materials - University of Oxford

- Ph.D. project on computational materials science:
  Optical properties of semiconductors at finite temperatures from first principles
  (with Prof. F. Giustino, Materials Modelling Laboratory)
- Courses attended:
  High performance computing on parallel architectures,
  Density functional theory, Symmetry in condensed matter physics
- Computational packages used: *Quantum Espresso, EPW, YAMBO*

10 October 2009 – 1 August 2013 – London, United Kingdom

MSci in Physics - University College London

- 1st class degree / **Ranked 1st** in the 2013 Physics cohort
- Final year project on computational materials science:
  Modeling doping in the transparent conducting oxide Ga_2O_3
  (with Prof. D. Bowler, London Centre for Nanotechnology)
- *Computational packages used: VASP*

TEACHING EXPERIENCE

1 September 2019 – present – Lemesos, Cyprus

Lecturer in Department of Mechanical Engineering and Materials Science, Cyprus University of Technology

- *Quantum Mechanics*
- *Solid State Physics*

18 October 2015 – 10 June 2018 – Oxford, United Kingdom

Tutor in Trinity College and Department of Materials, University of Oxford

- *Mathematics for Materials and Earth Sciences*
- *Partial Differential Equations and Fourier Series*

RESEARCH INTERESTS

First-principles methods; Solar cells; Perovskites; Static and time-resolved inelastic scattering; Photo-emission spectroscopy; Many-body perturbation theory; Parallel computing code development; Density functional theory; Electron-phonon coupling; Molecular dynamics; Excitonic effects; 2D materials; Renewable energy

RESEARCH GRANTS

- Computational Resources Grant for *trSCAPHOL,* PRACE DECI-17 call (4000 kCPUh), **1 Nov. 2021 – 1 Nov. 2022**
- Research Grant, *Design of graphene-based materials for Li-ion batteries,* program ΜΕΤΑΔΙΔΑΚΤΩΡ of the Cyprus University of Technology (€ 20,000), **1 April 2021 – 31 December 2021**
- Computational Resources Grant, *Time-resolved diffuse scattering and photoluminescence in 2D materials from first-principles* (809 kCPUh), Cyprus Institute, **1 April 2021 – 1 April 2022**
- Computational Resources Grant for *ai-GRALIB*, PRACE DECI-16 call, Saniyer at UHEM, (3930 kCPUh), **20 November 2020 – 20 November 2021**
- Research Grant, *Electronic transport in thermoelectric perovskites*, Max Planck Society, (€ 37,000 and access to MPCDF supercomputing services), **1 October 2018 – 1 January 2020**
- Computational Resources Grant for *T-DOPS*, National Supercomputer ARCHER, UK, (59.040 kAU ~ £ 40,000), **1 December 2017 - 1 December 2018**
- Academic Grant, Trinity College, Oxford, (£ 2,000), **10 December 2016**

RESEARCH ARTICLES / PUBLICATIONS

* Indicates publications for which the MZ is the corresponding author.

- M. Zacharias*, P. Kelires, *Quantum confinement of electron-phonon coupling in graphene quantum dots* The Journal of Physical Chemistry Letters 12, 9940, (2021)
- M. Zacharias*, H. Seiler, F. Caruso, D. Zahn, F. Giustino, P. C Kelires, R. Ernstorfer: *Efficient first-principles methodology for the calculation of the all-phonon inelastic scattering in solids* Physical Review Letters 127, 207401, (2021), **Editors' Suggestion**.
- M. Zacharias*, H. Seiler, F. Caruso, D. Zahn, F. Giustino, P. C Kelires, R. Ernstorfer: *Multiphonon diffuse scattering in solids from first-principles: Application to layered crystals and 2D materials* Physical Review B 104, 205109 (2021), **Editors' Suggestion**.
- H. Seiler, D. Zahn, M. Zacharias, P. Hildebrandt, T. Vasileiadis, Y. Windsor, Y. Qi, C. Carbogno, C. Draxl, R. Ernstorfer, F. Caruso, *Accessing the anisotropic non-thermal phonon populations in black phosphorus*, Nano Letters 21, 14 (2021)
  Contribution of MZ: Calculations of (i) All-phonon structure factors, (ii) non-equilibrium lattice dynamics
- L. Schade, S. Mahesh, G. Volonakis, M. Zacharias, B. Wenger, F. Schmidt, S. V. Kesava, D. Prabhakaran, M. Abdi-Jalebi, M. Lenz, F. Giustino, G. Longo, P. G. Radaelli, H. J. Snaith: *Crystallographic, optical, and electronic properties of the $Cs_2AgBi_{1-x}In_xBr_6$ double perovskite: ... photovoltaic efficiency challenges,* ACS Energy Letters 6, 3, 1073, (2021)
  Contribution of MZ: Band structure unfolding calculations of $Cs_2AgBi_{1-x}In_xBr_6$
- T. A. Huang, M. Zacharias, D. K. Lewis, F. Giustino, S. Sharifzadeh: *Exciton-phonon interactions in monolayer germanium selenide from first principles,*

The Journal of Physical Chemistry Letters, 2, 15, 3802 (2021)
Contribution of MZ: Special displacement and band structure unfolding at finite temperatures

- S. Park, H. Wang, T. Schultz, D. Shin, R. Ovsyannikov, M. Zacharias, D. Maksimov, M. Meissner, Y. Hasegawa, T. Yamaguchi, S. Kera, A. Aljarb, M. Hakami, L. Li, V. Tung, P. Amsalem, M. Rossi, N. Koch: *Temperature-dependent electronic ground state charge transfer in van der Waals heterostructures,*
  Advanced Materials, 2008677, (2021)
  Contribution of MZ: Monte Carlo approach for electronic structure calculations at finite temperatures
- F. Caruso, P. Amsalem, J. Ma, A. Aljarb, T. Schultz, M. Zacharias, V. Tung, N. Koch, C. Draxl: *Two-dimensional plasmonic polarons in n-doped monolayer MoS_2,*
  Physical Review B 103, 205152 (2021)
  Contribution of MZ: Band structure unfolding calculations of n-doped monolayer MoS_2
- V-A. Ha, G. Volonakis, H. Lee, M. Zacharias, F. Giustino: *Quasiparticle band structure and phonon-induced band gap renormalization of the lead-free halide double perovskite $Cs_2InAgCl_6$*
  The Journal of Physical Chemistry C 125, 21689 (2021)
- M. Zacharias and F. Giustino, *Theory of the special displacement ... structure calculations at finite temperature,*
  Physical Review Research 2, 013357, (2020)
- M. Zacharias*, M. Scheffler, C. Carbogno, *Fully anharmonic nonperturbative theory of vibronically renormalized electronic band structures*,
  Physical Review B 102, 045126, (2020)
- M. Zacharias*, P. Kelires, *Temperature dependence of the optical properties of silicon nanocrystals,*
  Physical Review B 101, 245122, (2020)
  Contribution of MZ: Special displacement method and band structure unfolding at finite temperatures
- R. P. Xian, V. Stimper, M. Zacharias, S. Dong, M. Dendzik, S. Beaulieu, B. Schölkopf, M. Wolf, L. Rettig, C. Carbogno, S. Bauer, R. Ernstorfer, *A machine learning route between band mapping and band structure*,
  arXiv:2005.10210 (2020), under peer-review.
  Contribution of MZ: All first-principles calculations for WSe_2
- M. A. Perez-Osorio, A. Champagne, M. Zacharias, G.-M. Rignanese, F. Giustino, *Van der Waals interactions and anharmonicity in the lattice vibrations, ... of the organic-inorganic halide perovskite $CH_3NH_3PbI_3$.*
  The Journal of Physical Chemistry C 121 (34), 18459, (2017)
  Contribution of MZ: (i) Calculation of the vibrational properties, (ii) investigation of anharmonicity
- M. Zacharias, F. Giustino, *One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization.*
  Physical Review B 94, 075125, (2016), **Editors' Suggestion**.
- M. Zacharias, C. E. Patrick, F. Giustino, *Stochastic approach to phonon-assisted optical absorption*,
  Physical Review letters 115, 177401, (2015)

CONFERENCE PRESENTATIONS

- **26-29 September 2021**
  Contributed Talk, XXXV Panhellenic Conference on Solid State Physics and Materials Science (virtual),
  Quantum confinement effects on the phonon-induced band gap renormalization of graphene quantum dots
- **20-23 September 2021**
  Contributed Talk, E-MRS Fall meeting (virtual),
  Quantum confinement effects on electron-phonon coupling in graphene quantum dots
- **6-9 July 2021 – Thessaloniki, Greece**
  Invited Talk, 18th International Conference on Nanosciences & Nanotechnologies (virtual),
  Quantum confinement effects on the phonon-induced band gap renormalization of graphene quantum dots
- **14-18 June 2021 – Austin, Texas, United states of America**
  Invited Lecture and Tutorial, Electron-Phonon Physics School and the EPW code (virtual)
- **16 February 2021 – Nicosia, Cyprus**
  Invited Talk, CaSToRC HPC National Competence Center Seminar Series, Cyprus Institute (virtual)
  Special displacement method for the calculation of materials' properties at finite temperatures
- **9 November 2020 – Boston, United States of America**
  Invited Talk, Sahar Sharifzadeh group, Boston University (virtual),

Temperature-dependent materials properties from first-principles using the ZG-package

- **28 September 2020 – Austin, Texas, United States of America**
  Invited Talk, EPW Developers' meeting (virtual),
  Implementation of the ZG package in EPW
- **23 September 2020 – Rennes, France**
  Invited Talk, Jacky Even group, Institut des Sciences Chimiques de Rennes (virtual),
  Temperature-dependent materials properties from first-principles
- **7-10 July 2020 – Thessaloniki, Greece**
  Invited Talk, 17th International Conference on Nanosciences & Nanotechnologies (virtual),
  Temperature dependence of the optical properties of silicon nanocrystals
- **21-25 June 2020 – Berlin, Germany**
  Contributed Talk, FHI-aims Developers' and Users' Meeting (virtual),
  Band structure unfolding using numeric atom-centered orbitals: An implementation in FHI-aims
- **2-4 April 2019 – Regensburg, Germany**
  Contributed Talk, DPG Spring Meeting,
  Temperature-dependent properties of solids using the ZG-configuration
- **22-24 May 2018 – Louvain-la-Neuve, Belgium**
  Contributed Talk, ETSF workshop on Electron-Phonon Interactions,
  Temperature-dependent optical spectra and band structures using the special displacement method
- **10-11 April 2017 – Cambridge, United Kingdom**
  Contributed Talk, CCP9 Conference and Young Researchers Event,
  First-principles calculation of temperature-dependent properties of semiconductors
- **13-17 May 2017 – New Orleans, United States**
  Contributed Talk, APS March Meeting 2017,
  One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization
- **6-10 June 2016 – London, United Kingdom**
  Contributed Talk, 13th ETSF Young Researchers' Meeting,
  Phonon-Assisted Optical Properties of Semiconductors
- **6-10 September 2015 – San Sebastian/Donostia, Spain**
  Poster, Psi-K Conference, *Stochastic approach to phonon-assisted optical absorption*

ORGANIZATION OF COLLOQUIA AND SEMINARS

- Theory Department Seminars, Max Planck Fritz-Haber-Institue, Berlin, Germany:
  Quantum Nuclear Effects in Thermal Transport, **6 May 2019**
  Towards interpretable machine learning for materials science, **8 February 2019**
  Calculation framework for reproducible science, **28 November 2018**
- Materials Modelling Laboratory Colloquia, University of Oxford, United Kingdom:
  Materials and devices for energy harvesting and storage, **9 February 2018**
  Materials for electronics and optoelectronics, **10 November 2017**

ONGOING COLLABORATIONS

- *Temperature-dependent optical properties of Lead-free Halide double Perovskites*
  Collaborators: Prof. F. Giustino (University of Texas at Austin)
- *Modelling of phonon and carrier nonequilibrium dynamics in 2D materials*
  Collaborators: Dr. F. Caruso (University of Kiel)
- *Optical properties of* $Cs_2AgBi_{1-x}In_xBr_6$ *double perovskite*
  Collaborators: Prof. H. J. Snaith (University of Oxford), Dr. G. Volonakis (University of Rennes 1)
- *Thermal and nonequilibrium vibrational dynamics in 2D materials*
  Collaborators: Prof. R. Ernstorfer (Max Planck Fritz-Haber-Institute in Berlin)
- *Exciton-phonon coupling in 2D materials via GW/BSE calculations and the special displacement method*
  Collaborators: Dr. S. Sharifzadeh (Boston University)

CODES DEVELOPED

- *disca code:* First-principles calculations of all-phonon inelastic scattering in solids.
  Distributed as part of EPW in Quantum Espresso (*github.com/QEF/q-e/releases*),
  Collaborators: Prof. R. Ernstorfer (Fritz-Haber-Institute) and Prof. F. Giustino (University of Texas at Austin)
- *ZG code:* Special displacement method for calculations of temperature dependent properties of solids.
  Distributed as part of EPW in Quantum Espresso (*github.com/QEF/q-e/releases*),
  Collaborators: Prof. F. Giustino (University of Texas at Austin)
- *Band structure unfolding using plane waves code:* Elestron spectral functions of materials.
  Distributed as part of EPW in *Quantum Espresso (github.com/QEF/q-e/releases),*
  Collaborators: Prof. F. Giustino (University of Texas at Austin)
- *Band structure unfolding using numeric atom-centred orbitals code:* Spectral function calculation and band unfolding of structures from ab-initio Molecular Dynamics. To be distributed as part of *FHI-aims,*
  Collaborators: Dr. C. Carbogno (Fritz-Haber-Institute), Prof. M. Scheffler (Fritz-Haber-Institute)

AWARDS AND HONOURS

- *EPSRC Doctoral Training Award,* University of Oxford, **14 October 2013 - 14 April 2017**
- *Graduate Prize for academic excellence,* Trinity College, Oxford, **10 November 2015**
- *Dean's list, Outstanding Performance in Physics ,* University College London, **1 August 2013**
- *Cyprus State Scholarships Foundation,* Cyprus , **September 2009 - September 2013**
- *38th International Physics Olympiad,* Isfahan, Iran, **7-16 July 2007**
- *Balkan Mathematical Olympiad,* Rhodes, Greece, **26 April - 2 May 2007**
- *Best Cypriot student in Mathematics,* University of Cyprus, **4 July 2007**
- *First prizes in Physics competition,* Cypriot Physicists Society, **2 July 2005, 3 July 2006, 4 July 2007**
- *First prizes in Mathematics competition,* Cypriot Mathematical Society, **3 July 2006, 4 July 2007**
- *47th International Mathematical Olympiad,* Ljubljana, Slovenia, **7-17 July 2006**
- *European Union Science Olympiad (EUSO),* Brussels, Belgium, **2-8 April 2006**

HIGH PERFORMANCE PARALLEL COMPUTING EXPERIENCE

- 1**4 October 2012 - 10 June 2013:** *Legion,* University College London, usage: > 100 kCPUh
- **14 October 2013 - 14 August 2018:** *ARC,* University of Oxford, usage: 3000 kCPUh
- **1 February 2017 - 10 December 2018:** *Cartesius,* Dutch National Supercomputing Service, usage: > 1000 kCPUh
- **1 December 2017 - 1 December 2018:** *ARCHER,* United Kingdom, usage: > 1000 kCPUh
- **1 October 2018 - 30 September 2020:** *MPCDF,* Germany, usage: > 4000 kCPUh
- **1 January 2019 - present:** *Cytera and Cyclone,* Cyprus Institute, usage: > 2000 kCPUh
- **11 October 2019 - 10 December 2019:** *Marconi-KNL,* CINECA, Italy, usage: 100 kCPUh
- **1 June 2020 - present:** *Stampede2,* Texas advanced computing center, usage: > 1000 kCPUh
- **20 November 2020 – present:** *Saniyer,* Uhem, Turkey, usage: 3000 kCPUh
  Codes compiled and used: *VASP, Quantum Espresso, EPW, FHI-aims, YAMBO*

OUTREACH ACTIVITIES

- *Native scientist:* Teaching science to kids between 5-7, The Orthodox Church, **14 January 2017**
- Committee member of the *Oxford University Greek Society*, **10 April 2015 - 10 April 2017**
  Organization of social events to raise money for the *Refugees crisis* in Greece
  Help in the organization of *Modern-Greek seminars, Greek dances*, and *drama plays of PRAXIS*

OTHER INFORMATION

- Software: Bash, Matlab, Python, FORTRAN, c++, Gnuplot, Vesta, Jmol, LaTeX, GitLab, Microsoft Office
- Languages: Greek (native), English (Proficient user)
- Travelling, Participating in social events, Networking, Basketball, Football, Music, Shotokan (1st dan)