[redacted]

05/01/2024
Formigine (MO)

Peter Gillespie

Dr Peter N O Gillespie
[redacted]
[redacted]

Overview

Postdoctoral research associate currently employed by the National Research Council of Italy (CNR), working on the development of techniques using the Python-based AiiDA software platform (https://www.aiida.net/) to develop automated workflows for the calculation of X-Ray Absorption spectra and to apply such techniques to the analysis of materials related to battery materials (see below for examples of code contributions).

From the research work I carried out in my masters and PhD degrees, I have both a firm understanding of and a strong interest in the electronic and spectroscopic properties of solid-state materials, in particular for those with potential applications in solar energy and energy storage technologies, and seek to focus on projects which investigate the structure-property relationships in materials.

Since finishing my PhD research I have taken these skills and augmented them by combining this knowledge with state-of-the art python-based automation techniques as part of my postdoctoral research. I highly value collaborative work between computational and lab-based researchers, and have a strong interest in projects that wish to use computational analysis to aid the design and engineering of functional materials.

Current and Previous Work Experience

Postdoctoral Research Fellow (December 2020 - *Present*)

- Role: Postdoctoral researcher reporting to Prof. Elisa Molinari and Dr Deborah Prezzi, employed as part of work package 2 (WP2) within the Battery Interface Genome Materials Acceleration Programme "BIG-MAP" (https://www.big-map.eu/) to develop automated workflows for calculations of XANES spectra with Quantum Espresso. (https://www.quantum-espresso.org/) using the AiiDA workflow engine.
- Organisation: National Research Council of Italy (CNR)
- Office Address: CNR-NANO-S3, Dipartimento di Scienze Fisiche, Informatiche, e Matematiche, Università degli studi di Modena e Reggio Emilia, Via Giuseppe Campi 213/A, Modena (MO), 41125

Code Development Projects

AiiDA-QE XANES Spectra Workflows

- Repository links (from github.com/aiidateam/aiida-quantumespresso/ project):
  - Workflows:github.com/aiidateam/aiida-quantumespresso/tree/main/src/aiida_quantumespresso/workflows/xspectra
  - Utility Functions: github.com/aiidateam/aiida-quantumespresso/tree/main/src/aiida_quantumespresso/calculations/functions/xspectra
- Modular workflow system written in Python for the Quantum Espresso module of AiiDA.
- Provides a complete automated workflow for the calculation of XANES spectra of a given input structure with Quantum Espresso, including automated job submission, management, post-processing, and automatic restart functionality from AiiDA.
- Modular & flexible workflow design enables users to utilise workflow components for more complex analysis

[redacted]
05/01/2024
Formigini (MO)

- Includes tools to assist with structure preparation & post-processing for XANES spectra.

AiiDALab-QE GUI Implementation of XANES Workflows

- Code under review, see pull request: (https://github.com/aiidalab/aiidalab-qe/pull/580)
- Complete GUI implementation of AiiDA-QE plugin for XANES spectra simulation for the AiiDALab-QE GUI program with simple, easy-to-use interface which exploits capabilities for automated input parameter setting without compromising robustness of final results.
- Includes interactive spectrum post-processing tools with breakdown of contributions from different absorbing atoms and data export for detailed analysis..

Education

University of Sheffield, South Yorkshire, UK

- Chemistry PhD, *December 2014 - January 2019*. Passed
- Thesis Title: Theory of Charge Transfer in Solar Energy Materials
- Subject of Research: Computational modelling of composites for solar energy applications. Research aims were to design a model to simulate a composite material of reduced graphene oxide (RGO) and titanium dioxide (TiO_2), a photocatalytic material studied experimentally in the past. The model we produced successfully demonstrated the critical role of oxygen functional groups in the interaction between RGO and TiO_2.

University of Surrey, Surrey, UK

- MRes Chemistry degree, *October 2013 - October 2014*. Graduated with Merit
- Subject of Research: Computational modelling of defects in radiation-damaged graphene. Research aims were to model the aggregation of defect carbon atoms on graphene surfaces, looking in particular at the stabilities of defect structures and the dynamics of the defect atoms themselves. The results showed multiple ways in which defect atoms could aggregate to form potential structures.

University of East Anglia, Norfolk, UK

- MChem Chemistry degree, *September 2009 - July 2013*. Graduated (classification 2.2)
- Final-Year Project: Computational modelling of a transition metal complex for use in luminescent materials

Farnborough Sixth-Form College, Hampshire, UK

- A-Level Chemistry (B)
- A-Level Mathematics with Statistics (C)
- A-Level Biology (C)
- A-Level Psychology (B)

Publications

- (In-Progress): Peter N. O. Gillespie, Michael A. H. Bertran, and Deborah Prezzi. *Automated Workflows for Core-Level Spectroscopy Simulation*

- (In-Progress): Antonella Iadecola, Quentin Jacquet, Sandrine Lyonnard, Nataliia Mozhzhukhina, Aleksandar Matic, Gilles Moehl, Lucia Perez, Jean-Pascal Rueff, Stephanie Belin, Federico Capone, Rémi Dedryvère, Lorenzo Stievano, Nicholas B. Brookes, Alessandro Longo, Peter Gillespie, and Deborah Prezzi. *Atomic and electronic structure of Li_xNiO_2 probed by multi - technique spectroscopies.*

- M. G. Betti, D. Marchiani, A. Tonelli, M. Sbroscia, E. Blundo, M. De Luca, R. Frisenda, C. Mariani, S. Jeong, Y. Ito, N. Cavani, R. Biagi, P. N. O Gillespie, M. A. H. Bertran, M. Bonacci, E. Molinari, V. De Renzi, D. Prezzi. *Dielectric Response and Excitations of Hydrogenated*

[redacted]

05/01/2024
Formigine (MO)

Free-Standing Graphene, Carbon Trends, 2023, 12, 100274 https://doi.org/10.1016/j.cartre.2023.100274

- P. N. O. Gillespie, and N. Martsinovich; *Origin of Charge Trapping in TiO_2 Reduced Graphene Oxide Photocatalytic Composites: Insights from Theory, J. Appl. Mater. Interfaces*, 2019, 11, 35, pp 31090-31922 https://pubs.acs.org/doi/10.1021/acsami.9b09235
- P. N. O. Gillespie, and N. Martsinovich; *Electronic Structure and Charge Transfer in the TiO_2 Rutile (110)/Graphene Composite Using Hybrid DFT Calculations; J. Phys. Chem. C*; 2017; 121 (8), pp 4158–4171 https://pubs.acs.org/doi/10.1021/acs.jpcc.6b12506

Additional Qualifications

- Strong skills in core Python programming and shell-scripting, with a good understanding of Python libraries such as AiiDA, SciPy, Pandas, Pyplot, and NumPy (examples available in code development projects section and GitHub page: https://github.com/PNOGillespie).
- Written and published two articles of original research, with two more currently in progress (see publications list), in addition to various code contributions to GitHub repositories for the AiiDA-QE and AiiDALab-QE projects (see code development projects section).
- Have given numerous poster and oral presentations of work done both during postdoctoral and PhD studies at various conferences (see conferences list).
- Good proficiency in spoken and written Italian, with 3 years experience living in Italy.
- Have carried out work as a lab demonstrator for physical chemistry over one year of the PhD, in addition to marking lab reports during that time.
- Have gained further experience in teaching through working independently as a tutor between February and September 2020, including an enhanced DBS background check.

[redacted]
05/01/2024
Formigine (MO)

Conferences

Oral Presentations

- 10th NANO Colloquia Sessions (2024), CNR-NANO-S3, Modena, IT
- Midlands Computational Chemistry Meeting (2017), University of Sheffield, South Yorkshire, UK
- Annual Northern Universities Meeting on Physical Chemistry (2017), University of Sheffield, South Yorkshire, UK
- Advanced Energy Materials (AEM) (2016), University of Surrey, Surrey, UK

Poster Presentations

- BIG-MAP 6th Project Meeting (2023), Solvay Campus, Brussels, BE
- Battery 2030+ Conference (2023), Uppsala University, Uppsala, SE
- 6th UK Solar Fuels Network Meeting (2018), University of York, North Yorkshire, UK
- 5th UK Solar Fuels Network Meeting (2017), University College London, Greater London, UK
- UK & Ireland SPS Meeting (2016), Tyndall Institute, Cork, Ireland
- 4th UK Solar Fuels Network Meeting (2015), University of Cambridge, Cambridgeshire, UK
- 12th Materials Chemistry Conference (2014), University of York, North Yorkshire, UK.

Referees

- Dr Natalia Martsinovich. Lecturer in physical chemistry. Office G2, Dainton Building, Brook Hill, Sheffield, UK, S3 7HF. Email: n.martsinovich@sheffield.ac.uk. LinkedIn: https://www.linkedin.com/in/natalia-martsinovich-68930920/
- Dr Garth Jones. Lecturer in physical chemistry. University of East Anglia, Norwich Research Park, Norwich, Norfolk, NR4 7TJ. Email: garth.jones@uea.ac.uk. LinkedIn: https://www.linkedin.com/in/garth-jones-a91b1a48/
- Dr Thomas Trevethan, CTO at CommerceBlock. Email: tptrevethan@googlemail.com. LinkedIn: www.linkedin.com/in/tomtrevethan.