# Geneviève Dusson

CNRS researcher at the Laboratoire de Mathématiques de Besançon, France.

*Laboratoire de Mathématiques*
*Université de Franche-Comté*
*Besançon, France*
✉ *g.dusson - at - math.cnrs.fr*
*gdusson.perso.math.cnrs.fr*

## Research Experience and Education

Feb. 2020-present **CNRS (Chargé de Recherche) research position**, *Laboratoire de Mathématiques de Besançon, Université Bourgogne Franche-Comté, France.*

Sept. 2019-Jan. 2020 **Tenure-track position**, *Laboratoire de Mathématiques de Besançon, Université Bourgogne Franche-Comté, France.*

2017-2019 **Post-doctorate**, *University of Warwick, United Kingdom.*
Subject: Development of **interatomic potentials** for molecular simulation with Christoph Ortner (Warwick) and Gábor Csányi (Cambridge).

2017 (3 months) **Research stay**, *Visit to Gero Friesecke, Technical University Munich, Germany.*
Subject: density to pair density map in electronic structure calculation.

2014 - 2017 **PhD in Applied Mathematics**, *Université Pierre et Marie Curie, Paris, France.*
- Title: **Error estimation** for linear and nonlinear **eigenvalue problems** arising from **electronic structure calculation**
- Advisors: Prof. Yvon Maday (Laboratoire Jacques-Louis Lions), Prof. Jean-Philip Piquemal (Laboratoire de Chimie Théorique).
- Defended on October 23, 2017.

2013 - 2014 **Master's degree in Applied Mathematics**, *Paris 6 University, France*, specialised in Numerical Analysis, Partial Differential Equations, obtained with Highest Distinction.

2010 - 2014 **Master's level engineering school**, Ecole Centrale Paris, France.

## Fellowships

- 2019: International Junior Fellowship in Mathematics: numerical analysis, scientific computing, and modeling, funded by ISITE-BFC.
- 2017 : Scholarship of the foundation Pierre Ledoux for a three-months research stay (awarded by the Fondation de Sciences Mathématiques de Paris) spent at the Technical University of Munich in collaboration with Gero Friesecke (March-June 2017).
- 2017 : SIAM Student Travel Award for the conference CSE17 (USA) in February 2017.

## Publications

1. Cas van der Oord, Geneviève Dusson, Gábor Csanyi, and Christoph Ortner, *Regularised atomic body-ordered permutation-invariant polynomials for the construction of interatomic potentials* ArXiv e-prints, 1910.06010. to appear in Machine Learning: Science and Technology (2019).
2. Eric Cancès, Geneviève Dusson, Yvon Maday, Benjamin Stamm, Martin Vohralík, *Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: a unified framework*, Nümerische Mathematik, 140(4), 1033–1079 (2018).
3. Eric Cancès, Geneviève Dusson, Yvon Maday, Benjamin Stamm, Martin Vohralík, *Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: conforming approximations*, SIAM Journal on Numerical Analysis, 55 (2017), pp. 2228–2254.
4. Eric Cancès, Geneviève Dusson, *Discretization error cancellation in electronic structure calculation: toward a quantitative study*, ESAIM: Mathematical Modelling and Numerical Analysis, 51 (2017), pp. 1617–1636.
5. Eric Cancès, Geneviève Dusson, Yvon Maday, Benjamin Stamm, Martin Vohralík, *A perturbation-method-based post-processing for the planewave discretization of Kohn–Sham models*, Journal of Computational Physics 307 (2016) 446–459.
6. Geneviève Dusson, Yvon Maday, *A Posteriori Analysis of a Non-Linear Gross–Pitaevskii type Eigenvalue Problem*, IMA Journal of Numerical Analysis (2016), drw001.
7. Eric Cancès, Geneviève Dusson, Yvon Maday, Benjamin Stamm, Martin Vohralík, *A perturbation-method-based a posteriori estimator for the planewave discretization of nonlinear Schrödinger equations*, Comptes Rendus Mathematique, 352 (2014), pp. 941–946.

## Teaching

Fall 2018 **Matrix Analysis and Algorithm**, *lectures for third year undergraduate students*, in charge of the module, (30h).

Summer 2018 **Summer school in mathematics and chemistry (Roscoff)**, *Practical sessions on optimisation with Python*, master's level, (15h).

2015-2016 **Videos: Quantum Chemistry: the basics**, Master's level, 5×30 min.
`https://www.youtube.com/channel/UCoj8rmlGqm0q-Gq-ujPFUgA`

2014-2015 2015-2016 **Analysis (differential equations, sequences, series, integrals), Linear Algebra**, *teaching assistant*, bachelor's level, (192h).

Summers 2013 and 2015 **Practical sessions in Scilab**, *Summer school in mathematics and chemistry (Roscoff)*, master's level, (25h).

## Side activities

January 2017 Co-organizer of a young researchers workshop day on mathematical methods in quantum chemistry funded through a BOUM project SMAI (corresponds to the french SIAM).

2016-2017 Representative of PhD students at the committee of Jacques-Louis Lions laboratory.

2015-2017 Co-creator and co-organizer of a math-chemistry lecture group for young researchers in Paris.

2014-2015 Organizer of a working group with PhD student and postdocs at ICS (Institute for Scientific Computing).

## Conference talks

- 9-10 December 2019, London, United Kingdom, ICL-CNRS Workshop on Interacting Particle Systems and Applications
  Title: *Interatomic Potentials from Symmetry-adapted Polynomials*
- 15-19 July 2019, Valencia, Spain, International Congress on Industrial and Applied Mathematics
  Titles: *Guaranteed a posteriori bounds for eigenvalues and eigenvectors: multiplicities and clusters* and *Atomic Permutation-Invariant Potentials (aPIPs): A potential for materials based on polynomial fits*
- 10-16 June 2019, Suzhou, China Workshop on Mathematical and Numerical Analysis of Electronic Structure Models
  Title : *Data-driven interatomic potentials based on symmetric polynomials*
- 24-26 April 2019, Göttingen, Germany, Workshop on Developing High-Dimensional Potential Energy Surfaces – From the Gas Phase to Materials
  Title : *Interatomic Potentials from Linear Polynomial Regression*
- 25 February-1 March 2019, Spokane, USA, SIAM conference: Computational Science and Engineering
  Title : *Permutation-invariant Interatomic Potentials Based on Ab-initio Data*
- 10-12 September 2018, Aachen, Germany, Franco-German Workshop on mathematical aspects in computational chemistry
  Title : *Permutation-Invariant Data-Driven Interatomic Potentials*
- 23-27 July 2018, Edimburgh, United Kingdom, Workshop on Particle-based methods in materials science
  Title : *Permutation-Invariant Data-Driven Interatomic Potentials*
- 18-24 March 2018, Oberwolfach, Germany, Workshop on Mathematical Methods in Quantum Chemistry
  Title : *An overview of a posteriori estimation and post-processing methods for nonlinear eigenvalue problems*
- 3-8 July 2017, Warwick, United Kingdom, Workshop on Density Functional Theory and Beyond: Analysis and Computation
  Title : *A posteriori error analysis and post-processing methods for linear and nonlinear eigenvalue problems*
- February 27- March 3, 2017, Atlanta, USA,
  Siam conference on computational science and engineering (CSE17), (minisymposium)
  Title of the talk: *Discretization error cancellation in electronic structure calculation*
- December 10-14, 2016, Xiamen, China, IMACS conference, (minisymposium)
  Title of the talk: *A posteriori error analysis for the planewave discretization of nonlinear Schrödinger equations*

- July 4-8, 2016, Roscoff, France, Workshop on Mathematical and Numerical Analysis of Electronic Structure Models
  Title of the talk: *A perturbation-method-based post-processing for the planewave discretization of Kohn–Sham models*
- February 22-26, 2016, Toronto, Canada, Workshop on Computation Of Quantum Systems In Cold-matter Physics And Chemistry
  Title of the talk: *A Posteriori Error Estimates for Nonlinear Schrödinger Equations*
- September 14-18, 2015, Ankara, Turkey, Enumath conference, (minisymposium)
  Title of the talk: *A Posteriori Error Estimates for Nonlinear Schrödinger Equations*
- June 7-10, 2015, Nantes, France, ADMOS Conference, (minisymposium)
  Title of the talk: *A posteriori Analysis for Nonlinear Eigenvalue Problems, Application to Electronic Structure Calculations*
- April 7-10, 2014, Berlin, Germany,
  Workshop on Mathematical and Numerical Analysis of Electronic Structure Models
  Title of the talk: *A Posteriori Analysis for the Gross-Pitaevskii equation.*