Théo Duez

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Born on 11 September 2000 – Based in Paris, France

Education

Oct 2024–Sep 2027
PhD in Applied Mathematics for Quantum Chemistry
CNRS - Cermics École Nationale des Ponts et Chaussés, Champs-Sur-Marne France
Supervisors: Éric Cancès and Mathieu Lewin

Sep 2020 – Sep 2024
Master of Science (Diplôme d'Ingénieur), Mathematics specialization
CentraleSupélec - Gif-sur-Yvette
Includes a gap year (Sep 2022 – Sep 2023) for research internships at CEA Paris-Saclay and the Max Planck Institute – see Work Experience

Sep 2023 – Sep 2024
Master 2 (M2), Analysis, Modelling and Simulation (AMS)
Université Paris-Saclay
Completed concurrently with the final year at CentraleSupélec

Sep 2021 – Jul 2022
Master 1 (M1), Fundamental Mathematics track
Université Paris-Saclay
Completed concurrently with CentraleSupélec; two courses taken at Saclay, remaining credits validated from CentraleSupélec coursework

Sep 2020 – Jul 2021
Bachelor's Degree, Mathematics
Université Paris-Saclay
Completed concurrently with the first year at CentraleSupélec

Sep 2018 – Aug 2020
Classes Préparatoires (CPGE), MP – option Informatique
Collège Stanislas, Paris

Awards

2023
Sophie Germain Excellence Scholarship
Fondation Mathématique Jacques Hadamard (FMJH)
Awarded for the Master's program in Mathematics and Applications, Université Paris-Saclay / Institut Polytechnique de Paris

Publications

2026
Geometric Time-Dependent Density Functional Theory
É. Cancès, T. Duez, J. van Gog, A. B. Lauritsen, M. Lewin, J. Toulouse
Physical Review Letters 136, 256401 — arXiv:2601.07724

2026 **Geometric Theory of Constrained Schrödinger Dynamics with Application to Time-Dependent Density-Functional Theory on a Finite Lattice**

É. Cancès, T. Duez, J. van Gog, A. B. Lauritsen, M. Lewin, J. Toulouse

Physical Review A 113, 062222 — arXiv:2601.07719

Work Experience

Apr 2024 – Aug 2024 **Research Intern**

Inria Paris & Cermics, Champs-sur-Marne, France

Supervisor: Éric Cancès

Apr 2023 – Aug 2023 **Research Intern**

Max-Planck Institute, Numerical Method for Plasma Physic department, Munich, Germany

Supervisor: Michael Kraus

Nov 2022 – Mar 2023 **Research Intern**

CEA Paris-Saclay, thermohydraulic and fluid mechanics team (STMF/LMSF), Saclay, France

Supervisor: Alain Cartalade

Nov 2020 – May 2022 **Research Training**

CentraleSupélec, Gif-sur-Yvette, France

Supervisor: Ludovic Goudenège

Teaching Experience

Apr 2026 – May 2026 **Partial Differential Equations: Variational Approaches**

École Nationale des Ponts et Chaussés — Undergraduate Year 3 — Lecture + Tutorials 12h

Reference professor: Frédéric Legoll

Jan 2026 – Apr 2026 **Analyse des EDPs (Distributions, Fourier Analysis, L^p Spaces)**

École Nationale des Ponts et Chaussés — Undergraduate Year 3 — Lecture + Tutorials 21h

Reference professor: Virginie Ehrlacher

Sep 2025 – Oct 2025 **Modeling with partial differential equations**

École Nationale des Ponts et Chaussés — Undergraduate Year 3 — Tutorials 7,5h

Reference professor: Tony Lelièvre

Apr 2025 – May 2025 **Partial Differential equations: Variational approaches**

École Nationale des Ponts et Chaussés — Undergraduate Year 3 — Lecture + Tutorials 18h

Reference professor: Frédéric Legoll

Jan 2025 – May 2025 **Supervision of a project of students**

École Nationale des Ponts et Chaussés — Undergraduate Year 3 — Supervision 12h

Sep 2024 – Nov 2024

Analyse des EDPs

École Nationale des Ponts et Chaussés — Undergraduate Year 3 — Lecture + Tutorials 20h

Reference professor: Virginie Ehrlacher — Substitute teacher

Sep 2021 – Apr 2022

Convergence, Integration, Probability and PDEs

CentraleSupélec — Undergraduate Year 3 — Tutorials 20h

Jul 2021

Teacher for the Summer School in Mathematics

CentraleSupélec — Undergraduate Year 2 — Tutorials 18h

Summer Schools

Sep 2025

Modern Wavefunction Based Methods in Electronic Structure Theory

University of Pisa - Pisa, Italia

May 2024

7th edition of the Mini-School Summer School for theoretical chemistry and physics

Laboratoire Jacques-Louis Lions - Paris, France

May 2024

6th edition of the Mini-School Summer School for theoretical chemistry and physics

Laboratoire Jacques-Louis Lions - Paris, France

Talks

Apr 2026

Illustration of the Geometric Principle in TDDFT with a 1D Soft-Coulomb Model

REGAL Workshop on the Foundations and Extensions of Density-Functional Theory - OsloMet, Oslo, Norway

Mar 2026

Constrained Schrödinger Dynamics and the Foundations of TDDFT

96th GAMM Annual Meeting - Stuttgart, Germany

Posters

Oct 2025

Accurate Ground State Computations of Atoms and Ions in Extended Kohn-Sham Theory

JuliaCon Local - CNAM, Paris

Sep 2025

Negative Atomic Ions In Extended Kohn-Sham Theory

Modern Wavefunction Based Methods in Electronic Structure Theory - University of Pisa, Italia

Conferences Attended

Sep 2024

Manuel Conference - Mathematical and Numerical Analysis of Electronic Structure Models

Stuttgart, Germany

Skills

Software

Julia, Git, C++, Python, MATLAB, LaTeX, Linux

Languages	French (native), English (C1), German (B1)

Interests

Sports	Running, Trail Running, Mountain Sports