Théo Cavignac

Post-doctoral researcher in Theoretical Chemistry and Material Modelling

theo.cavignac@proton.me
lattay.srht.site

Career objective

Pursuing academic research in the domain of material science using advanced modeling technics such as DFT and many-body approaches. Teaching a wide variety of subjects applicable to material science, from fundamentals of quantum mechanics and thermodynamics to advanced programming applied to numerical methods.

Experience and cursus

Sep. 2024 – Sep. 2026 **Post-doctoral research**, *Bochum, Germany*, Ruhr University Bochum (RUB), ICAMS/RC-FEMS
Participation to Simons collaboration on new frontiers in superconductivity as electronic structures modelling expert and Alexandria database project.

Mar. – Jun. 2024 **Post-doctoral research**, *Nantes, France*, CNRS, Institut des Matériaux Jean Rouxel de Nantes (IMN)
Modeling of luminescence from first principles in inorganic materials and developing related software.

Nov. 2020 – Nov. 2023 **PhD in Theoretical Chemistry**, *Nantes, France*, CNRS, IMN
Study of electronic and optical properties of defects in solids from first principles.

May – Oct. 2020 **Research internship**, *Nantes, France*, CNRS, IMN
Modeling luminescence of rare earth chalcogenides from first principles.

Jan. – Jul. 2019 **Software engineer internship**, *Louvain-la-Neuve, Belgium*, University of Louvain-la-Neuve, Institute of Condensed Matter and Nanosciences
Developing an alternative test suite infrastructure for ABINIT.

May – Nov. 2018 **Research engineer internship**, *Arpajon, France*, CEA (Atomic Energy Commission)
Reworking the parallelization of the DFT/DMFT interface in ABINIT

Sep. 2016 – Aug. 2020 **Centrale Lyon Engineering degree (MSc grade)**, *Ecully, France*, École Centrale Lyon, Generalist engineer

Sep. 2019 – Aug. 2020 **Master of Science in Nanoscale Engineering**, *Lyon, France*, École Centrale Lyon/University of Lyon, Complementary Master degree in nanoscale engineering

Skills

Languages	Native french speaker, fluent english speaker
Main scientific topics	Material chemistry, Electronic and optical properties of materials, Defect chemistry, Luminescence of solids
Soft skills	team work, leadership, mentoring, teaching, student supervision
Programming	Expert skills: Python, Lua, C; Advanced skills: Fortan 90, Go, C++, OCaml, Scheme; Intermediate skills: Julia, JavaScript
Computational chemistry software	Advanced skills: VASP, Phonopy, ASE; Intermediate skills: CRYSTAL, ABINIT; Beginner skills: Quantum-Espresso, Gaussian, CP2K, GPAW, DFTK.jl, LAMMPS
Office work	LaTeX, Beamer, Excel, Word, PowerPoint
Other	GNU/Linux system administration (Archlinux, Fedora, Debian, Ubuntu), Git and Github.com, participation to open source software projects

Scientific production

As of December 12, 2025, 8 published papers, 1 preprint, 6 public oral communications.

Publications

2025 *AI-Driven Expansion and Application of the Alexandria Database*, **T. Cavignac**, J. Schmidt, P. Breuck, A. Loew, T. Cerqueira, H. Wang, A. Bochkarev, Y. Lysogorskiy, A. Romero, R. Drautz, S. Botti, M. Marques, arXiv preprint

2025 *Machine-learning accelerated prediction of two-dimensional conventional superconductors*, T. Silva, **T. Cavignac**, T. Cerqueira, H. Wang, M. Marques, Mater. Horiz.

2024 *Neutral 2-phenylbenzimidazole-based iridium(III) complexes with picolinate ancillary ligand: tuning the emission properties by manipulating the substituent on the benzimidazole ring*, E. Martínez-Vollbert, C. Philouze, **T. Cavignac**, C. Latouche, F. Loiseau, P. Lanoë, Dalton Trans.

2024 *Luminescence Properties of Al_2O_3:Ti in the Blue and Red Regions: A Combined Theoretical and Experimental Study*, **T. Cavignac**, M. Vigier, E. Fritsch, P. Deniard, S. Jobic, C. Latouche, Inorg. Chem.

2023 *A computational study of $CaWO_4$: Raman spectrum, intrinsic defects, and excited state properties*, T. Ferré, **T. Cavignac**, S. Jobic, C. Latouche, Computational Materials Science

2023 *Shortwave UV Blue Luminescence of Some Minerals and Gems Due to Titanate Groups*, M. Vigier, E. Fritsch, **T. Cavignac**, C. Latouche, S. Jobic, Minerals

2022 *Modeling Luminescence Spectrum of $BaZrO_3$:Ti Including Vibronic Coupling from First Principles Calculations*, **T. Cavignac**, S. Jobic, C. Latouche, J. Chem. Theory Comput.

2022 *A Theoretical Discussion on the Stability of $(O_2)^-$ and $(S_2)^-$ Species in KCl and KBr Salts: Luminescence Spectra and Defect Energy Formation*, **T. Cavignac**, C. Latouche, S. Jobic, J. Phys. Chem. C

2020 *The Abinit project: Impact, environment and recent developments*, X. Gonze et. al., Computer Physics Communications

Oral communications

2025 *Ab Initio Computations and Data-Driven Insights for Material Discovery and Superconductors*, **T. Cavignac**, SPSSM 2025 (Nantes, France)

2023 *Accurate simulation of luminescence in inorganic solids*, **T. Cavignac**, Congrès SCF 2023 (Nantes, France)

2023 *Accurate simulation of luminescence in inorganic solids*, **T. Cavignac**, Journée de l'école doctorale 3MG (Nantes, France)

2022 *Accurate simulation of luminescence in inorganic solids*, **T. Cavignac**, Young Researcher Meeting or the European Theoretical Spectroscopy Facility (Marseille, France)

2022 *Accurate simulation of luminescence in inorganic solids*, **T. Cavignac**, Réunion du Groupe Français des Luminophores (Bordeaux, France)

2021 *Modeling luminescence porperties in solids: KCl:S and $BaZrO_3$ as test cases*, **T. Cavignac**, RFCT-PO Scientific meeting (Rennes, France)

Interests

Music	Rock (Hard-, Punk, Garage, Metal), Jazz, "Classical" (Moderne, Classical, Romantique), House, Rap, Reggae
Arts and crafts	Watercolor, Drumkit, DIY, 3D printing
Sports	Bouldering
Computer science	Programming languages design and implementation, Free and Open-Source Software, System level programming