Simon Thébaud

10750 Garden Crossing Way
37932 Knoxville, Tennessee
United States of America
✉ *thebaudsj@ornl.gov*

Thematics: Thermoelectric Materials, Thermal Materials, Resonant States, Disordered Materials, Nanostructured Materials, Alloys, Doped Semiconductors, Two-dimensional Materials, Electron Transport, Phonon Transport, Electron-Phonon coupling, Oxides, Graphene, Anderson Localization

Methods: Large-Scale Numerical Simulations, Density Functional Theory, Wannier Functions, Tight-Binding Models, Exact Diagonalization, Chebyshev Polynomial Green's Function Method, T-matrix Approximation

Education

2016–2019 **Ph.D. Theoretical Physics**, *Université Claude Bernard Lyon 1*, Lyon.
"Electron and phonon transport in disordered thermoelectric materials: dimensional confinement, resonant scattering and localization", supervisors: G. Bouzerar, Ch. Adessi

2015–2016 **MSc. Physics**, *Ecole Normale Supérieure de Lyon (ENSL)*, Lyon.
Grade A, 18.4/20, ranked 2/32
Courses on solid state physics, quantum mechanics, statistical physics, quantum fields...
"Effects of Resonant States on the Thermoelectric Properties in Doped Semiconductors", supervisor: G. Bouzerar

2014–2015 **Agrégation de Sciences Physiques**, *ENSL*, Lyon.
Ranked 6/1433 nationwide
High-level competition examination giving access to teaching positions

2013–2014 **MSc. Physics (1^{st} year)**, *ENSL*, Lyon.
Grade A, 17.6/20, ranked 3/43
"Magnetic Phases in Two-Dimensional Lattices of Correlated Fermions: Triangular Graphene Nanoflakes", supervisor: G. Bouzerar

2012–2013 **B.S. Physics**, *ENSL*, Lyon.
Grade A, 16.9/20, ranked 7/41
"Search for new physics in a final state X $\rightarrow$ HH $\rightarrow$ 4b", supervisor: M. Gouzevitch

Research Experience

2019– **Postdoctoral Researcher**, *Oak Ridge National Laboratory*, Oak Ridge, USA.
Study of vibrational properties, thermal transport, electron-phonon coupling and topological properties in materials for thermal management and other energy applications.

- Methodological studies of vibrational properties in disordered models and materials using the T-matrix approximation and the CPGF method [2]
- Electron-phonon interactions in Iridium using the Quantum Espresso and the EPW software [1]
- Study of twist dynamics and topological crossings in non-symmorphic materials
- Referee for Phys. Rev. B
- Organized the journal club of the Materials Theory, Modeling and Simulation section

2016–2019 **PhD Researcher**, *Institut Lumière Matière*, Lyon, France.

Study of resonant states, disorder and nanostructuring effects in thermoelectric materials using a combination of DFT calculations and tight-binding models

- DFT (SIESTA, Quantum Espresso, Phonopy) for electron and phonon band structures, extracting realistic tight-binding models
- Chebyshev-Polynomial Green's Function method for DOS, conductivity, spectral function in very large systems (exact treatment of disorder)
- Exact diagonalization for finite-size studies of IPR, diffusivity (exact treatment of disorder)
- Applications to resonant states, doping and confinement effects in Oxides [8][10][5], phonon properties in Graphene and Silicon [4]

2016 **Master's Researcher**, *Institut Lumière Matière*, Lyon, France.

Analytical and numerical calculations on the thermoelectric properties of resonant states [9]

2014 **Master's Researcher**, *Institut Lumière Matière*, Lyon, France.

Numerical calculations implementing the self-consistent Unrestricted Hartree Fock method to study itinerant magnetism in Graphene nanoflakes

2013 **Undergraduate Researcher**, *CERN*, Geneva, Switzerland.

Analyses of particle collision data from the CMS detector in search of new particles

Conferences, Schools and Workshop

May 2019 **EMRS Spring Meeting**, *Nice, France*.

Delivered a talk: S. Thébaud, Ch. Adessi, and G. Bouzerar, "Resonant states: from minimal model to Vanadium doping in Strontium Titanate"

May 2019 **Nanospain conference 2019**, *Barcelona, Spain*.

Featured in a talk: Ch. Adessi, S. Pecorario, S. Thébaud, and G. Bouzerar, "DFT Study of the transport properties of single layer MoS_2: Application to Thermoelectricity"

Oct. 2018 **Graphene & Co Research Group Annual Meeting**, *Sète, France*.

Featured in a talk: G. Bouzerar, S. Thébaud, S. Radescu and Ch. Adessi, "Phonon Lifetime and Thermal Properties in Irradiated Graphene"

Sept. 2018 **Summer School "Collective Behaviour in Quantum Matter"**, *International Center for Theoretical Physics, Trieste, Italy*.

Attended the three-week summer school and presented a poster: S. Thébaud, Ch. Adessi, and G. Bouzerar, "Effects of Resonant States, Localization and Nanostructuring on the Thermoelectric Properties"

Sept. 2018 **Trends in NanoTechnology 2018**, *Lecce, Italy*.

Featured in a talk: Ch. Adessi, S. Pecorario, S. Thébaud, and G. Bouzerar, "DFT Study of the Thermal Transport Properties of MoS_2: Application to Thermoelectricity"

Dec. 2017 **Laboratory Theoretical Conference**, *Lyon, France*.

Delivered a talk: S. Thébaud, Ch. Adessi, and G. Bouzerar, "Electronic Transport in Doped Oxides and Semiconductors: Application to Thermoelectricity and Spintronics"

Nov. 2017 **Thermoelectrics Research Group Annual Meeting**, *Montpellier, France*.

Delivered a talk: S. Thébaud, Ch. Adessi, S. Pailhès, and G. Bouzerar, "Resonant States, Quantum Confinement : Engineering Electronic Transport"

Jun. 2017 **Trends in NanoTechnology 2017**, *Dresden, Germany*.

Featured in a talk: Ch. Adessi, S. Thebaud, R. Bouzerar, and G. Bouzerar, "First Principle Investigation on Thermoelectric Properties of Transition Metal Dichalcogenides: Beyond Rigid Band Model"

May 2017 **EMRS Spring Meeting**, *Strasbourg, France*.
Delivered a talk: S. Thébaud, Ch. Adessi, S. Pailhès, and G. Bouzerar, "Boosting the Power Factor with Resonant States : a Model Study"

Nov. 2016 **Thermoelectrics Research Group Annual Meeting**, *Lyon, France*.
Delivered a talk: S. Thébaud, Ch. Adessi, S. Pailhès, and G. Bouzerar, "The Influence of Resonant States on Thermoelectric Properties"

Oct.-Dec. 2016 **Workshop on Scientific Computing**, *Lyon, France*.
Followed courses on system architecture, parallel programming, cluster usage...

Teaching Experience

2016–2019 **Teaching assistant**, *Université Claude Bernard Lyon 1*, Lyon, France.
Assisted in teaching undergraduate level courses during PhD work
- Led tutorial classes in **electromagnetism** (20h) and **solid state physics** (30h)
- Led practical work sessions in **thermodynamics** (20h) and **C++ programming** (90h)
- Prepared, led and graded weekly problem-solving sessions for small groups of 2-3 students in **thermodynamics** (30h)
- Prepared, supervised and graded oral and written partial examinations

2015-2016 **Teaching assistant**, *Lycée Jean Perrin*, Lyon, France.
Prepared, led and graded weekly problem-solving sessions for small groups of 2-3 students at the undergraduate level (40h)

2012-2013 **Tutor**, *Lycée Doisneaux*, Lyon, France.
- Performed volunteer work for the association "Trait d'union" which purports to help high-school students in low-income districts
- Tutored a class of high-school seniors for the Baccalaureat national examination

Skills and Interests

Languages

French Native

English Fluent

Spanish Basic

Leadership experience

2013 Lead organizer of a community event in Paris (300 attendees)

2013 Crew member for a community event in Manchester (1000 attendees)

2009-2010 Editor-in-chief of an online magazine on amateur audio drama

Computer skills

- Fortran programming
- C++ programming
- Parallel programming (MPI)
- Cluster usage
- LaTeX writing
- Inkscape, Audacity

Hobbies

- History and philosophy
- Tabletop and computer games including teamwork-based and investigation games

References

Postdoctoral Advisor

- Lucas Lindsay (Oak Ridge National Laboratory): lindsaylr@ornl.gov

PhD supervisors

- Georges Bouzerar (Institut Lumière Matière): georges.bouzerar@univ-lyon1.fr
- Christophe Adessi (Institut Lumière Matière): christophe.adessi@univ-lyon1.fr

Publications

[1] D. H. Moseley, S. Thébaud, L. R. Lindsay, Y. Cheng, D. L. Abernathy, M. E. Manley, and R. P. Hermann. **Temperature-dependent lattice dynamics in iridium.** *Phys. Rev. Mat.*, 4:113608, Nov. 2020.

[2] S. Thébaud, C. A. Polanco, L. Lindsay, and T. Berlijn. **Success and breakdown of the T-matrix approximation for phonon-disorder scattering.** *Phys. Rev. B*, 102:094206, Sept. 2020.

[3] Ch. Adessi, S. Thébaud, and G. Bouzerar. **First principle investigation of the influence of sulfur vacancies on the thermoelectric properties of single layered MoS_2.** *Phys. Chem. Chem. Phys.*, 22:15048, Jun. 2020.

[4] G. Bouzerar, S. Thébaud, S. Pecorario and Ch. Adessi. **Drastic effects of vacancies on phonon lifetime and thermal conductivity in graphene** *J. Phys.: Condens. Matter*, 32:295702, Apr. 2020.

[5] Ch. Adessi, S. Thébaud, and G. Bouzerar. **Ab initio investigation of the role of vanadium impurity states in $\mathbf{SrTiO_3}$ for thermoelectricity.** *J. Phys. Chem. Sol.*, 138:109180, Mar 2020.

[6] S. Thébaud, Ch. Adessi, and G. Bouzerar. **Investigating the high-temperature thermoelectric properties of n-type rutile TiO2.** *Phys. Rev. B*, 100:195202, Nov 2019.

[7] S. Thébaud, Ch. Adessi, and G. Bouzerar. **Large enhancement of the thermoelectric power factor in disordered materials through resonant scattering.** *Phys. Rev. B*, 99:245203, Jun 2019.

[8] G. Bouzerar, S. Thébaud, R. Bouzerar, S. Pailhès, and Ch. Adessi. **Absence of confinement in $(\mathbf{SrTiO_3})/(\mathbf{SrTi_{0.8}Nb_{0.2}O_3})$ superlattices.** *Phys. Rev. Materials*, 2:035402, Mar 2018.

[9] S. Thébaud, Ch. Adessi, S. Pailhès, and G. Bouzerar. **Boosting the power factor with resonant states: A model study.** *Phys. Rev. B*, 96:075201, Aug 2017.

[10] G. Bouzerar, S. Thébaud, Ch. Adessi, R. Debord, M. Apreutesei, R. Bachelet, and S. Pailhès. **Unified modelling of the thermoelectric properties in $\mathbf{SrTiO_3}$.** *EPL*, 118(6):67004, 2017.

[11] Ch. Adessi, S. Thebaud, R. Bouzerar, and G. Bouzerar. **First principle investigation on thermoelectric properties of transition metal dichalcogenides: Beyond the rigid band model.** *J. Phys. Chem. C*, 121(23):12577–12584, 2017.