



Luigi Ranalli

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Research Experience

University of Vienna - Computational Materials Physics

Vienna, Austria

ADVISOR: PROF. CESARE FRANCHINI

2021 - present

- Thesis: "Phonon Anharmonicity and Electronic Transport in the quantum paraelectrics KTaO_3 and SrTiO_3 "

University of Texas, Oden Institute

Austin, United State

HOST: PROF. FELICIANO GIUSTINO

2023 June - 2023 July

- Topic: Carriers mobility in STO mediated by machine learning predicted phonons

University of Bologna - Dept of Physics and Astronomy

Bologna, Italy

ADVISORS: PROF. CESARE FRANCHINI, PROF. MATTEO CALANDRA

2018 - 2021

- Thesis: "Computational study of the role of anharmonic phonon effects in the quantum paraelectric perovskite KTaO_3 "
- score: 110/110

University of Bologna - Dept of Physics and Astronomy

Bologna, Italy

ADVISOR: DR. TOBIAS CRAMER

2015 - 2018

- Thesis: "Characterization of elastic bio-electrodes based on nanostructured semiconductor polymer"
- score: 110/110

Publications

PUBLISHED

Cesare Tresca, Pietro Maria Forcella, Andrea Angeletti, **Luigi Ranalli**, Cesare Franchini, Michele Reticcioli, Gianni Profeta. "Evidence of Molecular Hydrogen in the N-doped LuH_3 System: a Possible Path to Superconductivity?". 10.48550/arXiv.2308.03619 (2023) - now accepted in Nature Communications

C. Verdi, **L. Ranalli**, C. Franchini, G. Kresse. "Quantum paraelectricity and structural phase transitions in strontium titanate beyond density functional theory". Physical Review Materials, 7, L030801 (2023)

L. Ranalli, C. Verdi, L. Monacelli, M. Calandra, G. Kresse, C. Franchini. "Temperature Dependent Anharmonic Phonons in Quantum Paraelectric KTaO_3 by First Principles and Machine Learned Force-Fields". Advanced Quantum Technologies, 10.1002/QUTE.202200131 (2023)

IN PREPARATION

L. Ranalli, C. Verdi, M. Zacharias, J. Even, F. Giustino, C. Franchini "Electron Mobilities in SrTiO_3 and KTaO_3 : Role of Phonon Anharmonicity, Mass Renormalization and Disorder". <https://arxiv.org/abs/2407.18771> (2024) . - under revision in Physical Review Materials

Presentations

CONTRIBUTED PRESENTATIONS AND POSTERS

L. Ranalli. 2024. Talk: "Mobility in SrTiO_3 Mediated by Machine Learning Predicted Anharmonic Phonons". Presented at: Deutsche Physikalische Gesellschaft (DPG), Technical University (TU), Berlin. (2024)

L. Ranalli, C. Verdi, L. Monacelli, M. Calandra, G. Kresse, C. Franchini. Poster: "Anharmonic phonons in quantum paraelectric KTaO_3 by machine learning assisted first principles calculations". Presented at: Psi-k Conference, Losanne, Switzerland. (2022)

L. Ranalli, C. Verdi, L. Monacelli, M. Calandra, G. Kresse, C. Franchini. Talk: "Machine Learning aided Phonon Anharmonicity: the Soft Mode in the Quantum Paraelectric KTaO₃". Presented at: APS March Meeting, Chicago, Illinois. (2022)

Awards, Fellowships, & Grants

2022 - .. **Doctoral Fellowship**, Vienna Doctoral School in Physics

Vienna

Teaching Experience

Summer

Semester **Advanced Electronic Structure**, Teaching Assistant

2024

*University of
Vienna*

Professional Development

2023 **EPW Summer School**, Electron-Phonon Physics from first principles

Austin

2022 **Machine Learning Summer School**, Focus on molecules and materials

Vienna

Mentoring

2024 **Zhu Yu**, as phd internship Co-supervisor

*University of
Vienna*

2023-2024 **Markus Schwarz**, as MS thesis Co-supervisor

*University of
Vienna*

2022 **Matteo Costa**, as BS thesis Co-supervisor

*University of
Bologna*

Service

2023 - 2024 **Vienna Doctoral School of Physics**, Student Representative

Vienna

2024 **Seminars on Computational Quantum Materials/University of Vienna**, Chair

Vienna

2023 **Seminars on Computational Quantum Materials/University of Vienna**, Chair

Vienna

Outreach

2023 **European Researchers Night**, VR for surface catalysis

Vienna

Skills

PROGRAMMING LANGUAGES

Intensive use : **PYTHON, SHELL SCRIPTING**

Moderate Use : **FORTRAN, C++, MATLAB**