# 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 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 LuH3 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"

## 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 Anarmonicity: 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* |
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## Teaching Experience

| Summer Semester 2024 | **Advanced Electronic Structure**, Teaching Assistant | *University of Vienna* |
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## Professional Development

| 2023 | **EPW Summer School**, Electron-Phonon Physics from first principles | *Austin* |
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| 2022 | **Machine Learning Summer School**, Focus on molecules and materials | *Vienna* |

## Mentoring

| 2024 | **Zhu Yu**, as phd internship Co-supervisor | *University of Vienna* |
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| 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* |
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| 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* |
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## Skills

PROGRAMMING LANGUAGES

Intensive use : **PYTHON**, **SHELL SCRIPTING**

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