

# I-Te Lu

"A computational materials physicist, hungry learner, problem finder and solver"

✉ i-te.lu@mpsd.mpg.de

🌐 www.linkedin.com/in/i-te-louis-lu

🏠 Building 99 (CFEL), O2.005, Luruper Chaussee 149, Hamburg 22761, Germany

📖 **Research Interests** (1) computational condensed matter theory (2) ultrafast dynamics in solid states (3) cavity-QED materials



## Education

- Sep 2014 – Jun 2020    📖 **PhD in Materials Science (Minor in Physics)**  
California Institute of Technology (Caltech), USA  
→ Thesis: *First-principles calculations of electron-defect interactions and defect-limited charge transport*  
→ Work as one of the main developers of PERTURBO, an open source code for electron-phonon interactions and carrier dynamics developed in Marco Bernardi's research group
- Sep 2010 – Jun 2012    📖 **MS in Applications of Synchrotron Radiation on Materials**  
National Synchrotron Radiation Research Center (NSRRC) and National Chiao Tung University (NCTU), Taiwan  
→ Thesis: *Synchrotron Radiation Infrared Ray Analysis of Human Lung Adenocarcinoma Living Cells Upon Exposure to Fe<sub>3</sub>O<sub>4</sub> and Fe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub> Nanomaterials*  
→ Characterize materials using synchrotron light beams, e.g., XAS, XPS and TXM
- Sep 2007 – Jun 2010    📖 **BS in Materials Science and Engineering**  
NCTU, Taiwan

## Work Experience

- Jul 2021 – present    📖 **Postdoctoral Research Fellow**, Prof. Angel Rubio's research group at Max Planck Institute for the Structure and Dynamics of Matter (MPSD)  
→ Develop quantum electrodynamics density functional theory (QEDFT) functionals for solid states materials
- Jul 2020 – Jul 2021    📖 **Postdoctoral Scholar**, Prof. Marco Bernardi's research group at Caltech  
→ Develop the subroutines for the interaction between electrons and defects in materials using first-principles methods
- Jul 2015 – Jun 2020    📖 **Research Assistant**, Prof. Marco Bernardi's research group at Caltech  
→ Investigate the interaction between electrons and defects in materials using first-principles methods and co-develop the open source code PERTURBO
- Aug 2013 – Jul 2014    📖 **Research Assistant**, Prof. Pu-Wei Wu's research group at NCTU  
→ Work on Pt catalysts for fuel cells

## Research Publications

- 1    **Lu, I.-T.**, Shin, D., De Giovannini, U., Hübener, H., Zhang, J., Latini, S., & Rubio, A. (2023). Time-based chern number in periodically driven systems in the adiabatic limit. *Phys. Rev. Res.*, 5, 013081.  
🔗 <https://doi.org/10.1103/PhysRevResearch.5.013081>
- 2    **Lu, I.-T.**, Zhou, J.-J., Park, J., & Bernardi, M. (2022). First-principles ionized-impurity scattering and charge transport in doped materials. *Phys. Rev. Mater.*, 6, L010801.  
🔗 <https://doi.org/10.1103/PhysRevMaterials.6.L010801>

- 3 **Lu, I.-T.**, Park, J., Zhou, J.-J., & Bernardi, M. (2020). Ab initio electron-defect interactions using wannier functions. *npj Computational Materials*, 6(1), 1–7. <https://doi.org/10.1038/s41524-020-0284-y>
- 4 Zhou, J.-J., Park, J., **Lu, I.-T.**, Maliyov, I., Tong, X., & Bernardi, M. (2020). Perturbo: A software package for ab initio electron-phonon interactions, charge transport and ultrafast dynamics. *arXiv preprint arXiv:2002.02045*. <https://arxiv.org/abs/2002.02045>
- 5 **Lu, I.-T.**, Zhou, J.-J., & Bernardi, M. (2019). Efficient ab initio calculations of electron-defect scattering and defect-limited carrier mobility [**Editors' Suggestion**]. *Physical Review Materials*, 3(3), 033804. <https://doi.org/10.1103/PhysRevMaterials.3.033804>
- 6 Martinolich, A. J., Lee, C.-W., **Lu, I.-T.**, Bevilacqua, S. C., Preefer, M. B., Bernardi, M., Schleife, A., & See, K. A. (2019). Solid-state divalent ion conduction in ZnPS<sub>3</sub>. *Chemistry of Materials*, 31(10), 3652–3661. <https://doi.org/10.1021/acs.chemmater.9b00207>
- 7 **Lu, I.-T.**, & Bernardi, M. (2017). Using defects to store energy in materials—a computational study. *Scientific Reports*, 7(1), 1–8. <https://doi.org/10.1038/s41598-017-01434-8>
- 8 **Lu, I.-T.**, Hsieh, Y.-C., Chen, P.-C., Wu, P.-W. Et al. (2015). EQCM study on pulse current Pt electrodeposition. *International Journal of Electrochemical Science*, 10(12), 10199–10209.
- 9 Chang, Y.-M., **Lu, I.-T.**, Chen, C.-Y., Hsieh, Y.-C., & Wu, P.-W. (2014). High-yield water-based synthesis of truncated silver nanocubes. *Journal of alloys and compounds*, 586, 507–511.
- 10 Lee, Y.-J., Hsieh, Y.-C., Tsai, H.-C., **Lu, I.-T.**, Wu, Y.-H., Ted, H. Y., Lee, J.-F., Merinov, B. V., Goddard III, W. A., & Wu, P.-W. (2014). Dealloyed Pt<sub>2</sub>Os nanoparticles for enhanced oxygen reduction reaction in acidic electrolytes. *Applied Catalysis B: Environmental*, 150, 636–646.
- 11 Kuo, C.-W., **Lu, I.-T.**, Chang, L.-C., Hsieh, Y.-C., Tseng, Y.-C., Wu, P.-W., & Lee, J.-F. (2013). Surface modification of commercial PtRu nanoparticles for methanol electro-oxidation. *Journal of power sources*, 240, 122–130.

## Certificates and Awards

- |                       |   |
|-----------------------|---|
| Oct. 2021 – Oct. 2023 | ■ Humboldt Research Fellowship, Germany   |
| Aug 2017              | ■ Argonne Training Program for Extreme-Scale Computing (ATPESC), USA<br>→ Selected participants are fully sponsored by Argonne National Lab to take a two-week intensive training on high-performance computing |
| Sep 2014 – Sep 2017   | ■ Government scholarship for USA study, Ministry of Education, Taiwan<br>→ Only one scholarship is awarded per year for Nanomaterials category  |
| Oct 2008 – Aug 2010   | ■ Stan Shih (Founder of Acer Inc.) Scholarship, Taiwan<br>→ The awarded students are encouraged to do community service   |

## Teaching and Mentoring Experience

- |                     |   |
|---------------------|---|
| May 2020 – May 2020 | ■ <b>Guest Lecture</b> on high performance programming (MPI/OpenMP), Caltech  |
| Jun 2019 – Aug 2019 | ■ <b>Mentoring an Undergraduate Student</b> in the Summer Undergraduate Research Fellowships program, Caltech             |
| Apr 2018 – Jun 2018 | ■ <b>Teaching Assistant</b> for "Computational Materials", APH/MS 256, graduate level course at Caltech                   |
| Jun 2017 – Aug 2017 | ■ <b>Mentoring Two Local Senior High School Students</b> on how to use Python and Raspberry Pi for a NSF project, Caltech |
| Oct 2016 – Dec 2016 | ■ <b>Teaching Assistant</b> for "States of Matters", APH/MS 105, graduate level course at Caltech                         |

## Teaching and Mentoring Experience (continued)

---

- |                     |   |
|---------------------|---|
| Feb 2012 – Jun 2012 | ■ <b>Teaching Assistant</b> for "Physical Metallurgy", NCTU   |
| Sep 2011 – Jan 2012 | ■ <b>Teaching Assistant</b> for "Applications of Synchrotron Accelerator Light Source", NSRRC   |
| Feb 2011 – Jun 2011 | ■ <b>Teaching Assistant</b> for "Elementary Materials Experiments", NCTU  |
| Jul 2009 – Feb 2010 | ■ <b>Mentoring a Local Senior High School Student</b> for an international science competition, and the student received 2 <sup>nd</sup> place in a poster presentation in the 2 <sup>nd</sup> APEC Future Scientist Conference in Thailand |