

## Tutorials on first principles calculations of materials properties—Part I

[in person (see locations below) and on zoom:

<https://uchicago.zoom.us/j/2975372052?pwd=S1FRK3BMc3dZVGQ4b1pSa3ZYNFIMUT09>]

The computational materials science center MICCoM (<https://miccom-center.uchicago.edu/>) is organizing a series of tutorials, the first part of which is given by members and collaborators of the Galli group (<https://galligroup.uchicago.edu/>) at the University of Chicago. The tutorials are meant to help incoming graduate students to familiarize themselves with methods and techniques utilized in first principles calculations of materials properties, encompassing heterogeneous materials, surfaces, interfaces and defects.

The tutorials may also be useful for advanced graduate students and post-doctoral researchers, including non-practitioners or experimentalists, who are interested in understanding basic concepts of first principles calculations.

The first part of these tutorials is focused on electronic structure and coherence properties of materials. The second part will be focused on dynamical properties.

**Wed., Nov 1, 2023      ERC 301B      3:30 pm – 5 pm**

Practical introduction to Density Functional Theory (DFT) and exchange energy functionals

Lecturer: Giulia Galli (<https://galligroup.uchicago.edu/People/galli.php>)

and Jiawei Zhan (<https://galligroup.uchicago.edu/People/jzhan.php>)

**Thur., Nov 2, 2023      ERC 201B      2 pm – 3:30 pm**

Introduction to calculations of electronic excited states carried out within many-body perturbation theory (GW, Bethe Salpeter Equation (BSE)) and time dependent DFT—part I

Lecturer: Marco Govoni (<https://marcogovoni.com/index.html>)

Yu Jin (<https://galligroup.uchicago.edu/People/yjin.php>)

Victor Yu (<https://galligroup.uchicago.edu/People/vyu.php>)

**Fri., Nov 3, 2023      ERC 301B      10 am – 11:30 am**

Calculations of electronic excited states carried out within many body perturbation theory (GW, Bethe Salpeter Equation (BSE)) and time dependent DFT—part II

Lecturer: Marco Govoni (<https://marcogovoni.com/index.html>)

Yu Jin (<https://galligroup.uchicago.edu/People/yjin.php>)

Victor Yu (<https://galligroup.uchicago.edu/People/vyu.php>)

**Thur., Nov 9, 2023      ERC 301B      10 am – 11:30 am**

Introduction to calculation of coherence times of defects in solids

Lecturer: Nikita Onizhuk (<https://galligroup.uchicago.edu/People/monizhuk.php>)

**Fri, Nov 10, 2023      ERC 301B      3:30 pm – 5 pm**

Introduction to quantum computing, with focus on Fermionic systems

Lecturer: Benchen Huang (<https://galligroup.uchicago.edu/People/bhuang.php>)