Tutorials on first principles calculations of materials properties—Part II

(in person (see locationss below) and on zoom:
https://uchicago.zoom.us/j/2975372052?pwd=S1FRK3BMc3dZVGQ4b1pSa3ZYNFlMUT09)

The computational materials science center MICCoM (https://miccom-center.uchicago.edu/) is organizing a series of tutorials. 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 should 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. Note however that there are two of the tutorials specifically devoted code development *(Jan 3rd and Jan 4th, 2024*).

This second series of tutorials is on coherence and electronic properties of materials, with emphasis on using simulation codes, specifically PyCCE (https://pycce.readthedocs.io/en/latest/index.html) and WEST (https://west-code.org/).

A third series of tutorials will start in March 2024 and will be on dynamical properties of materials.

Wednesday Jan. 3, 2024 **ERC 201B** **2:00 pm – 3:30 pm**
Developing the **PyCCE** code: how to modify and add to the package—Part I
Lecturer: Nikita Onizhuk (https://galligroup.uchicago.edu/People/monizhuk.php)

Thursday Jan. 4, 2024 **ERC 219** **2:00 pm – 3:30 pm**
Developing the **PyCCE** code: how to modify and add to the package—Part II
Lecturer: Nikita Onizhuk (https://galligroup.uchicago.edu/People/monizhuk.php)

Monday Jan. 22, 2024 **ERC 301B** **2:00 pm – 3:30 pm**
Using the **PyCCE** code to compute coherence properties of spin defects
Lecturers: Jonah Nagura (https://galligroup.uchicago.edu/People/jnagura.php)
Nikita Onizhuk (https://galligroup.uchicago.edu/People/monizhuk.php)

Thursday Jan. 25, 2024 **ERC 301B** **2:00 pm – 3:30 pm**
Introduction to **Quantum Defect Embedding Theory** (QDET) for the calculations of properties of spin defects in solids
Lecturers: Marco Govoni (https://marcogovoni.com/index.html)
Victor Yu (https://galligroup.uchicago.edu/People/vyu.php)

Wednesday Feb. 7, 2024 **ERC 301B** **9:00 am – 10:30 am**

Using the **WEST** code to compute electronic properties of solids and molecules (GW, BSE, QDET and TDDFT methods) – Part I

Lecturers: 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)

Wednesday Feb. 8, 2024 **ERC 201B** **10:00 am – 11:30 am**

Using the **WEST** code to compute electronic properties of solids and molecules (GW, BSE, QDET and TDDFT methods) – Part II

Lecturers: 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)

Some useful references:

PyCCE: A Python Package for Cluster Correlation Expansion Simulations of Spin Qubit Dynamic, Mykyta Onizhuk & Giulia Galli, Adv. Theory Simul. 2100254 (2021).

Excited state properties of point defects in semiconductors and insulators investigated with **time-dependent density functional theory**, Yu Jin, Victor Wen-zhe Yu, Marco Govoni, Andrew C. Xu, and Giulia Galli, J. Chem. Theory Comput. 19, 8689–8705 (2023).

Large scale **GW calculations**, Marco Govoni & Giulia Galli
J. Chem. Theory Comput. 11, 2680 (2015).

Implementation and Validation of Fully-Relativistic **GW Calculations**: Spin-Orbit Coupling in Molecules, Nanocrystals and Solids, Peter Scherpelz, Marco Govoni, Ikutaro Hamada, and Giulia Galli, J. Chem. Theory Comput. 12 (8), 3523-3544 (2016).

Finite-field approach to solving the **Bethe-Salpeter equation**, Ngoc Linh Nguyen, He Ma, Marco Govoni, Francois Gygi and Giulia Galli, Phys. Rev. Lett. 122, 237402 (2019).

Quantum Embedding Theories to Simulate Condensed Systems on Quantum Computers, Christian Vorwerk*, Nan Sheng*, Marco Govoni, Benchen Huang, and Giulia Galli,
Nat. Comput. Sci. 2, 424 (2022).

Green's function formulation of **quantum defect embedding theory**, Nan Sheng*, Christian Vorwerk*, Marco Govoni, and Giulia Galli, J. Chem. Theory Comput. 18, 3512 (2022).