FHI-aims *Tutorial Series 2021*

Properties of Materials from First Principles
A Virtual Hands-on Tutorial Using FHI-aims

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Beyond DFT in FHI-aims (RPA, GW, and BSE)

Schedule

Day 1

- Xinguo Ren: Random-phase approximation **(15:00 - 16:00)**
- Dorothea Golze: Excited State Formalisms for Charge Carriers / GW **(16:15 - 17:15)**
- Hands-on Tutorial: Setup-Session **(17:30 - 18:30)**

Day 2

- Recap of day 1 **(15:00 - 15:15)**
- Hands-on Tutorial: First Session **(15:15 - 16:45)**
- Hands-on Tutorial: Second Session **(17:00 - 18:30)**

Speaker 1

Xinguo Ren

Institute of Physics, Chinese Academy of Sciences, Beijing

Expert on electronic structure methods. His work has been focusing on developing and implementing the formalism of the random phase approximation (RPA) and the GW method, as well as their extensions, within the atomic orbital basis set framework. He has authored and co-authored over 60 scientific papers and delivered over 40 invited talks.

Speaker 2

Dorothea Golze

TU Dresden, Germany

Junior group leader working in the field of computational chemistry and physics. Current work focuses on the development of highly accurate methods for theoretical spectroscopy of materials and the implementation for massively parallel execution on high-performance computing platforms. Developer of CP2K and FHI-aims codes.

Hands-on Tutorial 2

GW, BSE, and RPA for molecules and solids

Hands-on Tutorial

Prerequisite

- For computationally light exercises we recommend a Linux/Mac OS computer/laptop with at least 2 cpu cores and 4GB of memory. However, computationally demanding exercises require access to one to few nodes of computing clusters.
- An installed and ready to use FHI-aims executable **version 210716_2**. The source code can be obtained from: **fhi-aims.org**
- To use provided tools alongside the tutorial, a **python3 (version 3.7>=)** installation on your machine is required
- For users who are not familiar with FHI-aims, it is strongly advised to study this introductory tutorial to obtain information regarding basics of running a simulation with FHI-aims:
  https://fhi-aims-club.gitlab.io/tutorials/basics-of-running-fhi-aims/

Hands-on Tutorial

How to Access The Tutorial Materials

- The instructions of the tutorial is openly available at:

  https://fhi-aims-club.gitlab.io/tutorials/rpa-and-gw-for-molecules-and-solids

- The complete solution files including input and output of simulations can be accessed through the tutorial repository:

  https://gitlab.com/FHI-aims-club/tutorials/rpa-and-gw-for-molecules-and-solids.git

- The communications between the participants and organizers are managed through the tutorials slack workspace. Please join and follow the workspace closely for latest news and updates:

  https://join.slack.com/t/fhiaimstutori-ypu5815

Hands-on Tutorial

Useful Tools

- Graphical Interface for Materials Simulations (GIMS)

   A browser-based, ready to use graphical user interface which can be used for various aspects of simulations with FHI-aims:

   https://gims.ms1p.org

- Command-Line Interface for Materials Simulations (CLIMS)

   It must be installed from the command-line terminal using `pip install clims` or on clusters `pip install --user clims`. Complete instructions are available at:

   https://gitlab.com/FHI-aims-club/utilities/clims

Hands-on Tutorial

Objectives

This tutorial introduces several Methods that go beyond the DFT level

- How to run GW, RPA and BSE calculations for solids and molecules with FHI-aims.
- How to interpret the results of the simulations and their meaning in the context of theoretical spectroscopy (e.g. photoemission and core level spectroscopy)
- Learn about the reference method RPA for benchmarking local and semi-local exchange-correlation functionals.

Hands-on Tutorial

Outline

- Basis sets for correlated methods
- Part 1: GW and BSE calculations for molecules
  a. GW eigenvalues and Photoemission
  b. Counterpoise Correction
  c. Core levels
  d. BSE
  e. Multiple GW solutions
- Part 2: RPA for solids
- Part 3: GW for solids
- Summary
- References

Hands-on Tutorial

Outline

Basis sets for correlated methods:

Information regarding the importance of basis set convergence in explicitly correlated methods, and current available basis set approaches in FHI-aims

GW eigenvalues and Photoemission:

Assessing the suitability of density-functional theory (DFT), Hartree-Fock (HF) and many-body perturbation theory (MBPT) in the GW approach for the calculation of electronic excitations, using the ethylene molecule C_2H_4 as the case study with the purpose of comparing the performance of different theoretical approaches with experimental photoemission spectra

Hands-on Tutorial

Outline

Counterpoise Correction:

Introducing the basis set superposition error (BSSE) and counterpoise correction approach to account for slow convergence of physical observable due to BSSE.

Core Levels:

Using GW method to calculate the core level of methanol molecule in the gas phase, and the ionization potentials (IPs) observed in x-ray photoemission spectroscopy

Hands-on Tutorial

Outline

BSE:

Studying neutral excitations on molecules using Bethe-Salpeter equation (BSE) as implemented in FHI-aims

Multiple GW solutions:

Studying solution behaviour of GW and how to address cases with multiple solutions using C2H4 molecule as the case study

RPA for solids:

Computing the electronic correlation energy by the Random-Phase Approximation (RPA), and perform stability analysis of rutile-TiO2 structure.

Hands-on Tutorial

Outline

GW for solids:

GW based band-structure calculations of Si-diamond structure

Summary:

Summary of the keywords needed to be set for RPA, GW, BSE calculations, as well as, information regarding available non-standard basis functions in FHI-aims which are helpful for reaching convergence in beyond-DFT methods

Hands-on Tutorial

Course

https://fhi-aims-club.gitlab.io/tutorials/rpa-and-gw-for-molecules-and-solids/

GW, BSE, and RPA for molecules and solids

| Home | → | **Just presented** (contains useful links for installing FHI-aims) |

| Part 1: GW and BSE for molecules | → | **Start here** (exercises can be run on a laptop) |

| Part 2: RPA for solids
Part 3: GW for solids | → | **Computationally expensive** (better to run on computer clusters) |

| Summary | → | Summary of important FHI-aims keywords used throughout the tutorial |

References

For more information regarding obtaining and installing FHI-aims, please look here:
https://fhi-aims-club.gitlab.io/tutorials/basics-of-running-fhi-aims/preparations/

Hands-on Tutorial

Tutors and how to reach us

Dorothea Golze

Yi Yao

Sixian Yang

Konstantin Lion

Levi Keller

Saeed Bohloul

Mohammad Nakhaee

Evgeny Moerman

Raise your voice on zoom or use the Slack workspace for questions