

PHYS-808

Summer School on Advanced Electronic Structure Theory in Condensed Matter Physics

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Cursus	Sem.	Type
Physics		Obl.

Language of teaching	English
Credits	1
Session	
Exam	Project report
Workload	30h
Hours	16
Courses	16
Number of positions	30

Frequency

Only this year

Remark

Next time: 08.07.2019 to 10.07.2019

Summary

This course covers various topics within the framework of density functional theory, including advanced energy functionals, electron-phonon interaction, electron correlation, description of excited states (GW, BSE, TDDFT), molecular dynamics, and machine learning approaches.

Content

In the last decades, Density Functional Theory (DFT) has emerged as a powerful tool to predict and understand the electronic properties of molecules, solids and liquids. However, in its simplest and widespread used formulation, DFT lacks an accurate description of many relevant physical quantities, including e.g. electron-electron interactions, dispersion forces and excitonic effects. The need of overcoming such limitations has triggered an intensive research effort, leading to the development of a plethora of distinct "beyond-DFT" approaches. Within this framework, our Summer School aims to overview some advanced techniques that have recently appeared in the spotlight of the electronic structure community.

Day 1 - Density Functional Theory: Strengths, Limits and Extensions

DFT handles the quantum many-body problem in terms of the ground state electron density. While conceptually exact, the explicit use of DFT in actual applications strongly depends on the quality of the approximate density functional employed. Our School will begin (Day 1) with a basic introduction to DFT, together with the reasons underlying its success and its practical implementations. Next, known drawbacks of (semi)local approximations to the exchange-correlation functional and possible solutions will be discussed. First, the hybrid Hartree-Fock/DFT method that allows to partially correct the self-interaction error will be considered. Second, non-local van der Waals methods will be introduced, in order to address non-local effects. Third, a Hubbard-corrected formalism of DFT (DFT+*U*), meant to cope with the over-delocalization problem, will be presented. Finally, methods for the description of the electron-phonon interaction in DFT calculations will be discussed.

Day 2 - Beyond DFT: GW, BSE, TD-DFT, RPA, MP2 and DMFT

As a ground state calculation, DFT is unable to accurately describe excitations. In order to solve this problem, novel first-principles methods have been proposed and they will be the focus of Day 2. On one hand, *quasi*-particle Green's function approaches - such as the GW and the Bethe-Salpeter equation (BSE) formalisms - are found to predict energy levels and optical excitations in good agreement with experiments. However, the large computational effort required to carry out such calculations has motivated a renewed interest in Time-Dependent Density Functional Theory (TD-DFT), as a powerful and less computationally expensive methodology rather than GW+BSE. Indeed, TD-DFT relies on density rather than on a multivariable Green's function and, also, it leads to a Dyson equation for a two-point - rather than a four-point (BSE) - interaction kernel. Nevertheless, improved TD-DFT kernels are necessary to reach accurate results. In this context, pros and cons of the GW and TD-DFT techniques will be compared, and efficient strategies to achieve high-quality electronic spectra combining the strengths of both approaches will be presented. Then, second order

Møller-Plesset perturbation theory (MP2) and the Random Phase Approximation (RPA) will be introduced in order to describe non-local dynamical electron correlation effects. Finally, Dynamical Mean Field Theory (DMFT) will be addressed for the description of strong electron correlation effects.

Day 3 - Molecular Dynamics and Machine Learning

Day 3 is devoted to the discussion of molecular dynamics (MD) and machine learning (ML) methods in the framework of the electronic structure theory. A thorough exploration of the phase space is often required in order to achieve a meaningful description of the system under investigation. This can be accomplished by studying the time-evolution of a system at finite temperatures and pressures. In this context, several flavors of MD simulations will be introduced. Firstly, we will consider the Born-Oppenheimer approach, in which it is assumed that the electronic and nuclear degrees of freedom are fully separable. Next, the more complex quantum MD approach attempts to simulate the full dynamics of both electronic degrees of freedom (quantum dynamics) and nuclear degrees of freedom (path integral MD). Finally, we will explore ML methodologies as new paradigms in computational condensed matter physics. Indeed, some ML tools, such as clustering or neural networks, promise exciting applications in the areas of classification, high-throughput materials searches and development of exchange-correlation functionals. Therefore, selected ML topics for electronic structure and material science applications will also be presented.

Keywords

DFT, electronic structure, electron-phonon interaction, GW, TDDFT, BSE, DMFT, correlation, hybrid functionals, van der Waals, DMFT, MD, machine learning

Resources

Websites

- <https://sites.google.com/view/eth-electronic-structure-2019/>