# Symposium Ab-Initio Approaches to Excitations in Condensed Matter (SYAI)

jointly organized by
Surface Science Division (O),
Thin Films Division (DS),
Semiconductor Physics Division (HL), and
Magnetism Division (MA)

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## Overview of Invited Talks and Sessions

(lecture room SCH 251)

### Invited Talks

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|---|---|---|---|---|
| SYAI 1.1 | Thu | 15:00–15:30 | SCH 251 | **Insights and Progress in Density Functional Theory** — Paula Paula Mori-Sanchez, Aron Cohen, •Weitao Yang |
| SYAI 1.2 | Thu | 15:30–16:00 | SCH 251 | **Quasiparticle energy calculations in a new light: from defects in semiconductors to the *f*-electron challenge** — •Patrick Rinke |
| SYAI 1.3 | Thu | 16:00–16:30 | SCH 251 | **LDA+DMFT approach to excitations spectrum in Half-Metallic Ferromagnets** — •Alexander Lichtenstein |
| SYAI 1.4 | Thu | 17:00–17:30 | SCH 251 | **Insight and prediction of material properties from ab initio calculations of electronic excitations** — •Lucia Reining, Matteo Gatti, Ralf Hambach, Christine Giorgetti |
| SYAI 1.5 | Thu | 17:30–18:00 | SCH 251 | **Local excitations in strongly interacting charge-transfer insulators: Frenkel excitons within TD-LDA+$U$ and strong coupling theory** — •Wei Ku |
| SYAI 1.6 | Thu | 18:00–18:30 | SCH 251 | **Electron tunneling and transport at molecular junctions** — •Roberto Car |

### Sessions

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|---|---|---|---|---|
| O 41.1–41.10 | Wed | 15:00–17:30 | SCH 251 | **Contributed Talks I** |
| O 42.1–42.126 | Wed | 17:45–20:30 | P2 | **Poster** |
| O 49.1–49.12 | Thu | 10:30–13:30 | SCH 251 | **Contributed Talks II** |
| SYAI 1.1–1.6 | Thu | 15:00–18:30 | SCH 251 | **Invited Talks** |
| O 67.1–67.6 | Fri | 11:15–12:45 | SCH 251 | **Contributed Talks III** |

# SYAI 1: Invited Talks

Time: Thursday 15:00–18:30 Location: SCH 251

**Invited Talk** SYAI 1.1 Thu 15:00 SCH 251

**Insights and Progress in Density Functional Theory** — Paula Paula Mori-Sanchez, Aron Cohen, and •Weitao Yang — Department of Chemistry, Duke University

Density functional theory of electronic structure is widely and successfully applied in simulations throughout engineering and sciences. However, there are spectacular failures for many predicted properties, which can be traced to the delocalization error and static correlation error of commonly used approximations. These errors include underestimation of the barriers of chemical reactions, the band gaps of materials, the energies of dissociating molecular ions and charge transfer excitation energies. Typical DFT calculations also fail to describe degenerate or near degenerate systems, as arise in the breaking of chemical bonds, and strongly correlated materials. These can all be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. The failure to describe the bandgaps in Mott insulators can also be traced to the violation of the combined condition for fractional charges and fractional spins. Understanding the errors of functionals in the simplest way possible — as violations of exact conditions for fractional charges and fractional spins – opens the path forward for reduction of the errors and for applications of density functional theory in new frontiers. [P. Mori-Sanchez, A. J. Cohen, and W. T. Yang, Phys. Rev. Lett. 100:146401(2008); Phys. Rev. B,77:115123(2008); J. Chem. Phys. 129:121104(2008); Science, 321:792(2008); arXiv:0809.5108]

**Invited Talk** SYAI 1.2 Thu 15:30 SCH 251

**Quasiparticle energy calculations in a new light: from defects in semiconductors to the $f$-electron challenge** — •Patrick Rinke — University of California at Santa Babara, CA 93106, USA

Focussing on spectroscopic aspects of semiconductors and insulators we will illustrate how quasiparticle energy calculations in the $G_0W_0$ approximation can be successfully combined with recent developments in density functional theory (DFT) to meet the challenges in the theoretical description of the electronic properties of these materials. For defects in semiconductors we present a new formalism that expresses their formation energy as successive charging of a configuration with unoccupied defects states. We demonstrate for the example of the self-interstitial in silicon that $G_0W_0$ overcomes the self-interaction and band-gap problem of the local-density approximation (LDA) to DFT and increases the formation energy of the neutral configuration by ∼1.1 eV. For group-III-nitrides and lanthanide oxides it proves necessary to remove or reduce the self-interaction already at the ground state level, which we achieve by using the exact-exchange optimized effective potential approach (OEPx) and a Hubbard-$U$ correction to the LDA, respectively. We demonstrate that the band parameters for group-III-nitrides derived from $G_0W_0$@OEPx are in very good agreement with the available experimental data and provide reliable predictions for all parameters which have not been determined experimentally so far. The good agreement of the $G_0W_0$@LDA+$U$ results with available experimental data for the lanthanide oxide series leads us to challenge the conventional view that regards these materials as strongly correlated.

**Invited Talk** SYAI 1.3 Thu 16:00 SCH 251

**LDA+DMFT approach to excitations spectrum in Half-Metallic Ferromagnets** — •Alexander Lichtenstein — Institute of Theoretical Physics, University of Hamburg, Germany

We present a realistic many-body approach to excitation spectrum in the itinerant magnetic systems. The Half-Metallic Ferromagnets are an important class of itinerant electron materials because of their potential for spin-electronics. The Heusler alloy NiMnSb was the first material predicted to be a Half-Metallic Ferromagnet(HFM)in the framework of the Local Density Approximation (LDA) with the Fermi level in the gap for one of the spin directions. We study the effects of strong correlation between spin and charge degrees of freedom in NiMnSb within the Dynamical Mean Field Theory (DMFT). Based on LDA+DMFT electronic structure calculations we present the first ab-initio evidence for the existence of non-quasiparticle states lying in the gap of the minority spin channel just above the Fermi level [1]. We discuss a general and exact scheme to spin-excitation spectrum in the magnetic nanosystems and investigate the temperature dependance of demagnetization in Half-Metallic Ferromagnets.

[1] M. I. Katsnelson, V. Yu. Irkhin, L. Chioncel, A. I. Lichtenstein, and R. A. de Groot, "Half-metallic ferromagnets: From band structure to many-body effects", Rev. Mod. Phys. 80, 315 (2008).

**30 min. break**

**Invited Talk** SYAI 1.4 Thu 17:00 SCH 251

**Insight and prediction of material properties from ab initio calculations of electronic excitations** — •Lucia Reining[1,2], Matteo Gatti[1,2], Ralf Hambach[1,2], and Christine Giorgetti[1,2] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility

The knowledge of the electronic response of a material to a perturbation allows one to derive spectra such as absorption or electron energy loss, and to describe correlation effects such as the screening of the hole left by the photoelectron in a photoemission experiment.

We will discuss the role of dynamical screening in theory (within the frameworks of many-body Green's functions and of density-functional based approaches) and in experiment. We will review fundamental ideas, possible combinations, interpretation of experimental results, and limitations. Various aspects will be illustrated with recent theoretical results such as the plasmon dispersion in carbon nanostructures [1], or photoemission spectra of transition metal oxides [2].

[1] C. Kramberger et al., Phys Rev. Lett. **100**, 196803 (2008); R. Hambach et al. Phys. Rev. Lett. (in press).

[2] M. Gatti et al., Phys. Rev. Lett. **99**, 266402 (2007)

**Invited Talk** SYAI 1.5 Thu 17:30 SCH 251

**Local excitations in strongly interacting charge-transfer insulators: Frenkel excitons within TD-LDA+$U$ and strong coupling theory** — •Wei Ku — Brookhaven National Lab, Upton, NY 11973, USA — Physics Department, Stony Brook University, Stony Brook, NY 11794, USA

Recent theoretical developments to better understand strongly bound local Frenkel excitations in "charge-transfer insulators" will be presented. First, the use of symmetry-respecting first-principles Wannier functions will be demonstrated to unify the description of charge-transfer insulators with the Mott insulators. Second, formal theoretical framework of TD-DFT with LDA+$U$ will be developed and applied to a case study illustrating its capability and deficiency. Third, systematic framework of strong coupling approach will be presented to account for the multiplets beyond the typical solutions of Bethe-Salpeter equation. Finally, a two-particle hopping kernel is introduced to describe propagation of the local excitations. Case studies include anisotropy of local excitations in NiO[1] and space-time propagation of excitons in LiF[2].

[1] B. Larson et al, Phys. Rev. Lett. 99, 026401 (2007).
[2] P. Abbamonte et al, Proc. Natl. Acad. Sci. 105, 12159 (2008).

**Invited Talk** SYAI 1.6 Thu 18:00 SCH 251

**Electron tunneling and transport at molecular junctions** — •Roberto Car — Princeton University, Princeton, NJ 08544, USA

In this talk I will review recent progress on the theory of electron transport through molecular junctions. Under weak bias conditions this problem can be effectively formulated within linear response theory. In the case of non-resonant tunneling this approach leads to a simple formula that can be applied to interpret the conductance of long molecular chains measured in recent experiments. I will also discuss a kinetic formulation of quantum transport which is valid under more general bias conditions. This approach illustrates the interplay between ballistic and dissipative effects in molecular electronics. Finally, I will comment on the use of density functional theory in transport problems.