Ab-initio correlated methods in spectroscopy

Monday 6. February 2017

Chair: J. Minár

9:00 - 9:10 Introductory remarks (practical information)

9:10- 9:40 Lucia Reining

A direct approach to the calculation of many-body Green's functions: Theoretical spectroscopy beyond quasi-particles

9:40-10:10 Marco Grioni

Experimental studies of correlated materials by ARPES and resonant inelastic x-ray scattering (RIXS)

10:10-10:40 Sergey Artyukhin

Magnetoelectric coupling through the spin flop transition in Ni3TeO6

10:40-11:10 Coffee Break

Chair S. Biermann

11:10-11:40 Alexander Shick

Racah materials: role of atomic multiplets in intermediate valence systems

11:40-12:10 Jan Kuneš

Spectroscopic signatures of excitonic magnetism

12:10-13:40 Lunch

Chair: V. Strocov

13:40-14:10 Silke Biermann

First principles calculations for correlated materials: Rethinking the interface between electronic structure and many-body theory

14:10-14:40 Andrivo Rusidy

High-energy optical conductivity on oxides interfaces and correlated electron systems

14:40-15:10 Coffee Break

Chair: M. Lüders

15:10-15:40 Micael Oliveira

Data exchange concepts for electronic structure codes within the CECAM electronic structure library

15:40-16:40 Discussions about formats for self energy and basis functions

18:00- Conference Dinner

Workgroup meeting supported by COST Action MP1306 EUSpec and by the CEDAMNF project CZ.02.1.01/0.0/0.0/15_003/0000358 of the Ministry of Education, Youth and Sports (Czech Republic).

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Tuesday 7. February 2017

Chair: J. Kuneš

9:00- 9:30 Malte Schüler
Influence of non-local interactions on the Mott metal-insulator transition

9:30-10:00 Jan Tomczak
Theoretical spectroscopies of correlated materials

10:00-10:30 Igor di Marco
DMFT and spectroscopy: from transition metals compounds to elemental lanthanides

10:30-11:00 Coffee Break

Chair J. Honolka

11:00-11:30 Jindřich Kolorenč
Core-level spectra in the dynamical mean-field theory

11:30-12:00 Vladimir Strocov
Electrons and polarons at oxide interfaces

12:00-13:30 Lunch

Chair: C. Draxl

13:30-14:00 Dimitrii Nabok
Accurate all-electron G0W0 quasiparticle energies employing the full-potential augmented planewave method

14:00-14:30 Christian Vorwerk
Correlation effects in core-level spectroscopy

14:30-15:00 Karel Výborný
Ellipsometry matches ab initio calculated optical properties: band structure confirmed?

15:00-15:30 Coffee Break

Chair: O. Šipr

15:30-16:00 Alberto Marmodoro
Selected aspects of NL-CPA

16:00-16:30 Sergey Mankovsky
Thermal effects in electronic structure

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Wednesday 8. February 2017

Chair: I. di Marco

9:00- 9:30 Francesco Sottile

Theoretical Spectroscopy: new frontiers for photoemission and inelastic X-ray scattering

9:30-10:00 Jan Honolka

XMCD of single atoms and clusters on surfaces: physisorbed and chemisorbed cases

10:00-10:30 Anna Taranukhina

Multichannel multiple scattering in the real-space Green's function formalism: Description of electron-hole correlation effects in XAS

10:30-11:00 Coffee Break

Chair A. Shick

11:00-11:30 Mark van Schilfgaarde

QSGW + magnetic DMFT, and its application to Ni

11:30-12:00 Peter Koval

G0W0 using localized basis sets: a benchmark for molecules

12:00-13:30 Lunch

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