

Program

Sunday, October 29, 2017

17:00 – 21:00 Registration

18:00 *DINNER*

Monday, October 30, 2017

08:00 *BREAKFAST*

09:00 – 09:10 Organizers

Introduction

Chair: Roser Valenti

09:10 – 09:40 Silke Biermann

**Ab initio calculations for correlated
electron materials in the 21st century**

09:40 – 09:50 *Discussion*

09:50 – 10:20 Alexander Lichtenstein

**Realistic many-body approach to
materials with strong nonlocal
correlations**

10:20 – 10:30 *Discussion*

10:30 – 10:50 Stephen Winter

**Dynamics of Kitaev magnets: From
ab-initio to experiments**

10:50 – 10:55 *Discussion*

10:55 – 11:20 *COFFEE BREAK*

Program

Monday, October 30, 2017

Chair: Bernhard Keimer

- 11:20 – 11:50 James Allen **DFT, DMFT and ARPES: Quest for convergence on hard problems**
- 11:50 – 12:00 *Discussion*
- 12:00 – 12:30 Ole Krogh Andersen **The Q-representation; do electronic correlations make the Fermi surface of CaVO₃ more cubic?**
- 12:30 – 12:40 *Discussion*
- 12:40 **Conference Photo** (in the front of the lecture hall)
- 12:50 *LUNCH*

Chair: Igor I. Mazin

- 14:30 – 15:00 Ryotaro Arita **Cluster multipole theory for functional antiferromagnets**
- 15:00 – 15:10 *Discussion*
- 15:10 – 15:40 Ferdi Aryasetiawan **Reinterpretation of spectral functions of correlated materials according to self-consistent GW+DMFT**
- 15:40 – 15:50 *Discussion*
- 15:50 – 16:20 Josef Kudrnovsky **A unified approach to physical properties of complex solids**
- 16:20 – 16:30 *Discussion*
- 16:30 – 17:00 *COFFEE BREAK*

Chair: Tanusri Saha Dasgupta

- 17:00 – 18:30 **Oral teasers** (2 min/poster)
- 19:00 *DINNER*

Program

Tuesday, October 31, 2017

08:00 *BREAKFAST*

Chair: Giovanni B. Bachelet

09:00 – 09:30 Alessandro Toschi **Dynamics of the magnetic moments in correlated metals: The case of Fe and Ni from ambient to Earth's core conditions**

09:30 – 09:40 *Discussion*

09:40 – 10:00 Sergey Streltsov **FeO₂: a possible novel magnetic constituent of Earth's lower mantle**

10:00 – 10:05 *Discussion*

10:05 – 10:35 Vaclav Drchal **Fluctuating magnetic moments in the Earth's core**

10:35 – 10:45 *Discussion*

10:45 – 11:10 *COFFEE BREAK*

Chair: Ole K. Andersen

11:10 – 11:40 Eva Pavarini **Understanding strongly correlated Ruthenates - spin-orbit and tetragonal coulomb tensor effects**

10:40 – 11:50 *Discussion*

11:50 – 12:20 Maurits Haverkort **Dynamics and correlation functions in complex quantum materials**

12:20 – 12:30 *Discussion*

12:30 *LUNCH*

Program

Tuesday, October 31, 2017

Chair: Lilia Boeri

14:30 – 15:00 *Sashi Satpathy*

Doping and strain effects on the electronic structure of the strong spin-orbit coupled Iridate Sr₂IrO₄

15:00 – 15:10 *Discussion*

15:10 - 15:40 *Indra Dasgupta*

Spin orbit induced emergent magnetic phases in Iridium based oxides

15:40 – 15:40 *Discussion*

15:50 – 16:20 *Markus Aichhorn*

Spin-orbit coupling and strong correlations: From materials to models

16:20 – 16:30 *Discussion*

16:30 – 18:30 *COFFEE and posters*

18:30 *DINNER*

Program

Wednesday, November 1, 2017

08:00 *BREAKFAST*

Chair: Ali Alavi

09:00 – 09:30 Paul J. Kelly **Finite temperature spin transport from fully relativistic scattering theory**

09:30 – 09:40 *Discussion*

09:40 – 10:10 Vladimir Antropov **Spin fluctuations and their influence on the electronic structure of metals**

10:10 – 10:20 *Discussion*

10:20 – 10:40 Geoffroy Hautier **Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining**

10:40 – 10:45 *Discussion*

10:45 – 11:10 *COFFEE BREAK*

Chair: Michele Parrinello

11:10 – 11:40 George Albert Sawatzky **Atomic correlation contributions to the effective mass, band gaps and bond lengths in transition metal and rare earth compounds**

10:40 – 10:50 *Discussion*

11:50 – 12:20 Ali Alavi **Quantum chemistry approaches to spin energetics in cuprates and porphyrins**

12:20 – 12:30 *Discussion*

12:30 *LUNCH*

Program

Wednesday, November 1, 2017

Chair: Claudia Felser

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| 14:30 – 15:00 | Jens Kortus | Fermi-Löwdin-Orbital based self-interaction-correction and Linnett double quartet theory |
| 15:00 – 15:10 | <i>Discussion</i> | |
| 15:10 – 15:40 | Walter Lambrecht | Lattice polarization effects on the GW band structure of strongly ionic materials |
| 15:40 – 15:50 | <i>Discussion</i> | |
| 15:50 – 16:20 | Michelle Johannes | Understanding the electrochemistry of batteries using physics and DFT |
| 16:20 – 16:30 | <i>Discussion</i> | |
| 16:30 – 16:45 | Stefan Jorda | About the Wilhelm and Else Heraeus Foundation |
| 16:45 – 18:30 | <i>COFFEE and posters</i> | |
| 19:00 | <i>DINNER</i> | |

Program

Thursday, November 2, 2017

08:00 *BREAKFAST*

Chair: George A. Sawatzky

09:00 – 09:30 Claudia Felser **Weyl semimetals**

09:30 – 09:40 *Discussion*

09:40 – 10:10 Sergey Savrasov **High surface conductivity of Fermi Arc electrons in Weyl semimetals**

10:10 – 10:20 *Discussion*

10:20 – 10:40 Philipp Hansmann **Unconventional Chiral superconductivity induced by long-range interaction**

10:40 – 10:45 *Discussion*

10:45 – 11:10 *COFFEE BREAK*

Chair: Alexander Lichtenstein

11:10 – 11:30 Christoph Heil **Ab initio calculation of anisotropic multigap superconductivity in the vicinity of a charge density wave in NbS₂**

11:30 – 11:35 *Discussion*

11:35 – 11:55 José A. Flores Livas **Cutting edge structure prediction and in silico materials design of superconductors**

11:55 – 12:00 *Discussion*

12:00 – 12:30 Mark van Schilfgaarde **Metal-insulator transition in copper oxides induced by apex displacements**

12:30 – 12:40 *Discussion*

12:40 *LUNCH*

Program

Thursday, November 2, 2017

Chair: Michelle Johannes

14:30 – 14:50 Ying Li **Microscopic modeling of optical conductivity in frustrated magnets**

14:50 – 14:55 *Discussion*

14:55 – 15:25 Bernhard Keimer **High-resolution spectroscopy of high-temperature superconductors**

15:25 – 15:35 *Discussion*

15:35 – 16:05 Michele Parrinello **Fluctuations, entropy and rare events**

16:05 – 16:15 *Discussion*

16:15 – 16:45 *COFFEE*

Chair: Lilia Boeri

16:45 – 17:15 Volker Heine **From then to now: a brief history of our subject in my life**

17:15 – 17:25 *Discussion*

17:25 – 17:40 **Poster Awards**

18:30 *HERAEUS DINNER*
(social event with cold & warm buffet with complimentary drinks)

Chair: Tanusri Saha Dasgupta

20:15 **Social evening**

Program

Friday, November 3, 2017

08:00 *BREAKFAST*

Chair: Sashi Satpathy

09:00 – 09:30 Olle Eriksson **Correlated electronic structures**

09:30 – 09:40 *Discussion*

09:40 – 10:10 Alexander Yaresko **Band structure origin of bi-quadratic
exchange interaction in Fe pnictides**

10:10 – 10:20 *Discussion*

10:45 – 10:45 *COFFEE BREAK*

Chair: Mojmir Šob

10:45 – 11:15 Andrei Postnikov **Dispersion interactions and competing
structures in III-VI layered
semiconductors**

11:15 – 11:25 *Discussion*

11:25 – 12:10 Organizers **Closing and final remarks**

12:10 *LUNCH*

End of the seminar and departure

NO DINNER for participants leaving on Saturday morning