## Program

### Sunday, October 29, 2017

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<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>17:00</td>
<td>Registration</td>
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<tr>
<td>18:00</td>
<td>Dinner</td>
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### Monday, October 30, 2017

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Speaker</th>
<th>Topic</th>
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<tr>
<td>08:00</td>
<td>Breakfast</td>
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<tr>
<td>09:00 – 09:10</td>
<td>Organizers</td>
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<td>Introduction</td>
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<td></td>
<td>Chair: Roser Valenti</td>
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<tr>
<td>09:10 – 09:40</td>
<td>Silke Biermann</td>
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<td>Ab initio calculations for correlated electron materials in the 21st century</td>
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<td>09:40 – 09:50</td>
<td>Discussion</td>
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<td>09:50 – 10:20</td>
<td>Alexander Lichtenstein</td>
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<td>Realistic many-body approach to materials with strong nonlocal correlations</td>
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<td>10:20 – 10:30</td>
<td>Discussion</td>
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<td>10:30 – 10:50</td>
<td>Stephen Winter</td>
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<td>Dynamics of Kitaev magnets: From ab-initio to experiments</td>
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<td>10:50 – 10:55</td>
<td>Discussion</td>
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<td>10:55 – 11:20</td>
<td>Coffee Break</td>
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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
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  FeO$_2$: 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
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
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
Wednesday, November 1, 2017

*Chair: Claudia Felser*

14:30 – 15:00 Jens Kortus  
Fermi-Löwdin-Orbital based self-interaction-correction and Linnett double quartet theory

15:00 – 15:10 *Discussion*

15:10 – 15:40 Walter Lambrecht  
Lattice polarization effects on the GW band structure of strongly ionic materials

15:40 – 15:50 *Discussion*

15:50 – 16:20 Michelle Johannes  
Understanding the electrochemistry of batteries using physics and DFT

16:20 – 16:30 *Discussion*

16:30 – 16:45 Stefan Jorda  
About the Wilhelm and Else Heraeus Foundation

16:45 – 18:30 *COFFEE and posters*

19:00 *DINNER*
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
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
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