

Program of the International CECAM-Workshop
“Correlated electron physics beyond the Hubbard model”
Bremen Center for Computational Materials Science – BCCMS
University of Bremen, February 4th - 8th 2019
Conference site: House of Science, Downtown

Monday, February 4th 2019 (Radisson Blu Hotel Bremen)

18:00 – 21:00 Registration

Tuesday, February 5th 2019 (House of Science Bremen, Downtown)

08:00 – 08:50 Registration

08:50 – 09:00 Opening and welcome, Tim O. Wehling

Session: Dynamical Mean Field Theory and diagrammatic extensions thereof

Chair: Andrew Millis

09:00 – 09:40 Philipp Werner, University of Fribourg, Switzerland
GW+DMFT simulation of lattice models in and out of equilibrium

09:40 – 10:20 Alexander I. Lichtenstein, University of Hamburg, Germany
Nonlocal correlated effects in magnetic materials

10:20 – 10:50 Coffee Break

10:50 – 11:30 Erik van Loon, University of Bremen, Germany
Dual boson approach to spatial correlations

11:30 – 12:10 James P. F. LeBlanc, Memorial University of Newfoundland, St. John's, Canada
Hubbard-like models: challenges and solutions via analytic treatments of numerical problems

12:10 – 12:15 Group Photo

12:15 – 13:50 Lunch Break (Restaurant Q1) and Coffee

Session: Quantum Cluster Approaches

Chair: Silke Biermann

13:50 – 14:30 Johannes Lischner, Imperial College London, United Kingdom
Many-body perturbation theory beyond GW

14:30 – 15:00 Coffee Break

15:00 – 15:40 André-Marie S. Tremblay, University of Sherbrooke, Québec, Canada
Antagonistic effects of nearest-neighbor repulsion on the superconducting pairing dynamics in the doped Mott insulator regime

15:40 – 16:20 Round Table Discussion
Diagrammatic and cluster extensions of DMFT: where are we?

18:20 Pickup to Welcome Reception (The Bremen Town Musicians, the statue near the town hall)

18:30 – 21:30 Welcome Reception (Bremen Town Hall)

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Wednesday, February 6th 2019 (House of Science Bremen, Downtown)

- Session:** **Coupled cluster, FCIQMC and related quantum chemical approaches**
Chair: Philipp Werner
- 09:00 – 09:40** Lucas K. Wagner, University of Illinois at Urbana-Champaign, Illinois, USA
Model Hamiltonians from ab-initio quantum Monte Carlo calculations
- 09:40 – 10:20** George Booth, University of Cambridge, United Kingdom
‘Static’ mean-field theory, ‘Dynamical’ mean-field theory, and ‘Static Dynamical’ mean-field theory
- 10:20 – 10:50** **Coffee Break**
- 10:50 – 11:30** Silke Biermann, Ecole Polytechnique, Palaiseau, France
Non-local interactions and non-local correlations: examples of dynamical mean field calculations for realistic materials
- 11:30 – 12:10** Tianyu Zhu, California Institute of Technology, Pasadena, California, USA
Correlated Green’s functions in materials: towards an ab initio treatment of the Kondo problem
- 12:10 – 13:50** **Lunch Break (Restaurant Q1) and Coffee**
- Session:** **Constrained many-body perturbation theory, density functional theory and related methods I**
Chair: Shan-Wen Tsai
- 13:50 – 14:30** Matteo Cococcioni, Swiss Federal Institute of Technology, Lausanne, Switzerland
Ab initio modeling of transition metal compounds using the extended DFT+U+V with self-consistent Hubbard parameters
- 14:30 – 15:10** Ferdi Aryasetiawan, Lund University, Sweden
The impact of long-range interaction on the electronic structure of correlated materials
- 15:10 – 15:50** Malte Rösner, Radboud University, Nijmegen, The Netherlands
cRPA simulations of layered materials
- 15:50 – 16:20** **Coffee Break**
- 16:20 – 17:00** Ryotaro Arita, University of Tokyo, Japan
Self-energy variational approach to correlated electron systems
- 17:00 – 17:40** Malte Schüler, University of Bremen, Germany
The Peierls-Feynman variational principle: applications to the extended Hubbard model and real materials

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- 17:40 – 18:20 Round Table Discussion**
Towards real materials: all ab-initio versus hybrid approaches in the wave function, Green function and density functional domain
- 18:40 Bus Pickup to Conference Dinner** (Radisson Blu, Wachtstraße)
- 19:00 – 22:30 Conference Dinner** (Restaurant Juergenshof)

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Thursday, February 7th 2019 (House of Science Bremen, Downtown)

- Session: Lattice Quantum Monte Carlo**
Chair: Johannes Lischner
- 09:00 – 09:40** Stefan Wessel, RWTH Aachen University, Germany
Nonlocal density interactions in auxiliary-field quantum Monte Carlo simulations
- 09:40 – 10:20** Thomas Devereaux, Stanford University, California, USA
Metallic transport, CDWs, and pairing without quasiparticles in the Hubbard model
- 10:20 – 10:50** **Coffee Break**
- 10:50 – 11:30** Andrew Millis, Flatiron Institute, City of New York, New York, USA
Ground-state properties of the hydrogen chain, and beyond
- 11:30 – 12:10** Sandro Sorella, International School for Advanced Studies (SISSA), Trieste, Italy
New insights in the sign problem within the auxiliary field quantum Monte Carlo technique
- 12:10 – 13:50** **Lunch Break (Restaurant Q1) and Coffee**
- Session: Diagrammatic Monte Carlo**
Chair: Ryotaro Arita
- 13:50 – 14:30** Boris Svistunov, University of Massachusetts Amherst, Massachusetts, USA
Polynomial complexity despite the fermionic sign
- 14:30 – 15:10** Nikolay Prokofiev, University of Massachusetts Amherst, Massachusetts, USA
Dirac liquids and interacting topological insulators by Diagrammatic Monte Carlo
- Session: Functional Renormalization Group**
- 15:10 – 15:50** Sabine Andergassen, University of Tübingen, Germany
Multiloop functional renormalization group for response functions
- 15:50 – 16:30** Shan-Wen Tsai, University of California Riverside, California, USA
Effects of retardation in the renormalization group approach to interacting fermions
- 17:25** **Poster Mounting**
- 17:30 – 21:00** **Poster Session + Catering Buffet (House of Science)**

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Friday, February 8th 2019 (House of Science Bremen, Downtown)

Session:	Constrained many-body perturbation theory, density functional theory and related methods II <i>Chair: Tim O. Wehling</i>
09:00 – 09:40	Carsten Honerkamp, RWTH Aachen University, Germany <i>Effective interactions from cfRG</i>
09:40 – 10:20	Alexander Steinhoff, University of Bremen, Germany <i>GW+T-Matrix approach to the excitonic Mott transition</i>
10:20 – 10:50	Coffee Break
10:50 – 11:30	Mark van Schilfgaarde, King’s College London, United Kingdom <i>QSGW+DMFT: accurate, nearly ab initio many-body treatment of strong correlations</i>
11:30 – 12:30	Concluding Round Table Discussion <i>How to approach correlated materials with non-local interactions realistically: next steps</i>
12:30 – 12:45	Closing words and Departure