Discussion sessions

Evaluation and planning





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Evaluation and planning

Bottom up approach

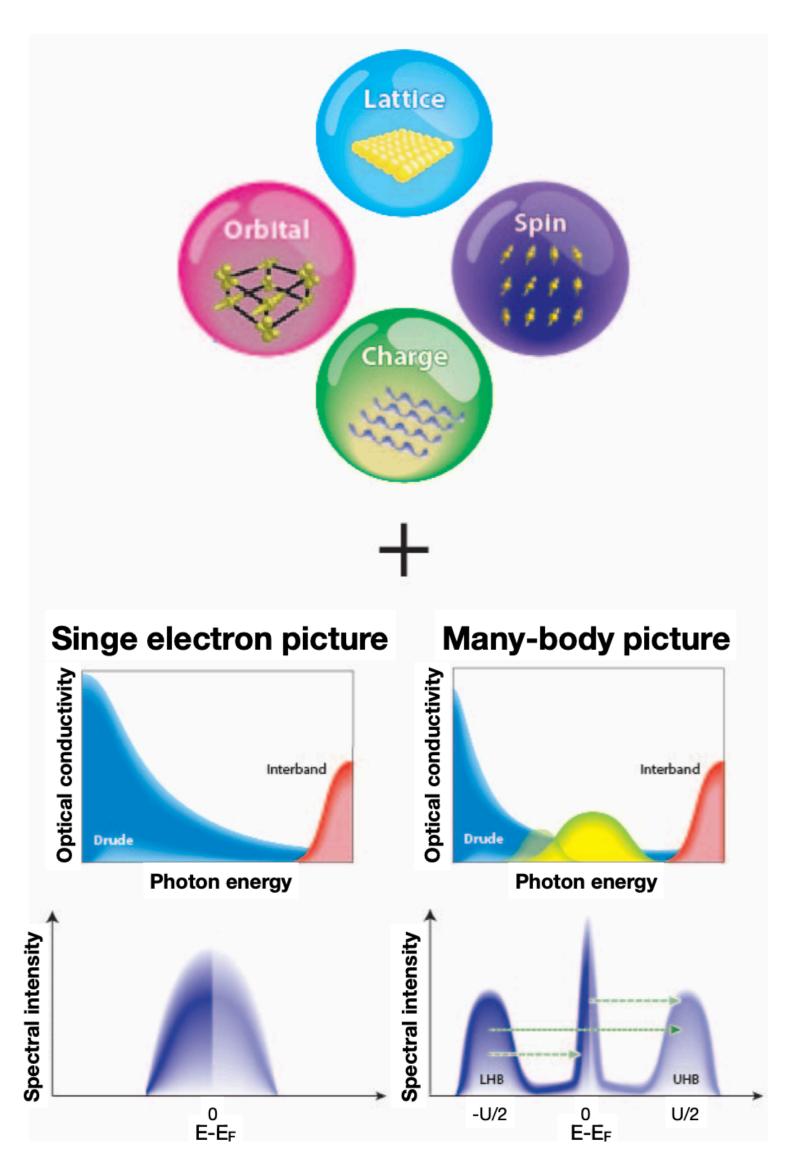
- **Day 1)** Discuss progress **so far** in smaller groups. Browse *abstract* (page 1) and *Important challenges* (page 2) of B1. If needed, check e.g. B2 for what methods we planned to use. Consider your work the past 3 years, how did we progress to meet these challenges. Consider to use the attached (auto-generate) list of publications acknowledging FASTCORR. Summarize in a few sentences and mail to <u>oscar.granas@physics.uu.se</u>.
- **Day 2)** What Assuming the fundamental questions are equally important today, consider B2 of the proposal (dated 2018!). What seems to be the best **way forward** in terms of theoretical/computational developments? What experiments are suitable for benchmarking these developments? Is anything lacking (identify needs)? Summarize in a few sentences and mail to <u>oscar.granas@physics.uu.se</u>.
- **Day 3)** Planning for upcoming work! Tightened collaborations, travel, next meeting etc.

FASTCORR

Excerpts from abstract

- Development of theory for driven quantum many-body systems that goes well beyond existing methods.
- This will be accomplished by developing dynamical mean-field theory and its generalizations, e.g., the dual fermion and dual boson theory, to cover out-of-equilibrium phenomena.
- We aim to create a solid theoretical foundation on which we will build practical tools. This involves:
 - (i) the development of fundamental mathematical and physical concepts,
 - (ii) software implementation
 - (iii) numerical simulations that will be compared to experiments.

Work packages



- WP1) Fundamental aspects
 PI Katsnelson
- WP2) Practical implementations and efficient algorithms
 PI Lichtenstein
- WP3) Materials simulations and connection to experiments PI Eriksson

What does a report contain?

Specify any major challenges, if any, you have encountered to date or anticipate in the near future related to the implementation of your research project, including any specific challenges linked to the implementation of the Synergy collaboration. Where appropriate, indicate any changes of direction you envisage.

Day 1

Evaluation of previous work

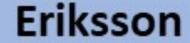
- Short summary of progress to meet FASTCORR challenges
- If any, use the attached (auto-generate) list to connect to publications (use number for reference)
- Significant challenges, anything missing? Funding? Infrastructure? (time is obvious)
- E-mail to oscar.granas@physics.uu.se.

Working groups Day 1

Patrik (Uppsala)
 DMFT, impurity models, exact diagonalization approach to spectroscopy etc

- Andrey (Nijmegen)
 Fundamental theory, complexity, aDS/CFT, etc
- Heike (Uppsala)
 Data-mining for correlated materials
- Evgeny & Hugo (Hamburg/Örebro) Dual fermions/Bosons, NEGF etc

Oscar (Uppsala)
 TD-DFT, Ehrenfest dynamics, transient spectroscopy



Calculations of properties, connection to experiment



74 high impact journal papers, 26400 citations; H-index 80

41465 citations H-index 97

Lichtenstein
Computational
methods,
theoretical
implementations

Katsnelson
Fundamental
theory,
mathematical
physics



132 high impact journal papers, 87100 citations; H-index 102

139108 citations H-index 128



62 high impact journal papers, 29600 citations; H-index 77

46767 citations H-index 96

Day 2 Preparatory planning

- What approach is the best way forward? (theory/computational)
- What experiments are suitable for benchmarking these developments?
- Overlap with the other FASTCORR nodes?
- E-mail to oscar.granas@physics.uu.se.

Day 3

Concrete planning for the coming years

- Projects to undertake
- Collaboration with other nodes
- Travel/exchange
- Next meeting
- E-mail to oscar.granas@physics.uu.se.