

Program of the 2nd Midterm Workshop
Research Training Group
„Quantum Mechanical Materials Modelling - QM³“
October 28th - 30th 2019

Conference site: Schloss Etelsen, Bremer Straße 2, 27299 Langwedel-Etelsen

Each project has allocated 45 minutes (30+15)

Round tables: “Quo vadis”-discussions ~ 45 min. Where are we? Which new topics to be addressed? How to strengthen collaborations in RTG?

Monday, October 28th 2019

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|--------------|----------|--------------|---|
| 09:00 | – | 10:00 | Registration at the registration desk |
| 10:00 | – | 10:15 | Opening and welcome, Thomas Frauenheim and Tim Wehling |
| 10:15 | – | 11:00 | Guest talk: Nonequilibrium materials design - from dynamical Hubbard U to optical control in 2D materials
<u>Dr. Michael Sentef (MPI Hamburg)</u> |
| 11:00 | – | 11:30 | Coffee Break |
| 11:30 | – | 12:15 | Guest talk: Ta ₂ NiSe ₅ - An excitonic insulator?
<u>Dr. Malte Rösner (Radboud University, Nijmegen)</u> |
| 12:15 | – | 13:30 | Lunch |
| 13:30 | – | 14:15 | P2: Many-body instabilities in 2D materials
<u>Jan Berges (University of Bremen)</u> |
| 14:15 | – | 15:00 | P3: Many-body approaches to realistic quantum impurity models and Coulomb engineering
<u>Edin Kapetanovic, (University of Bremen)</u> |
| 15:00 | – | 15:30 | Coffee Break |
| 15:30 | – | 16:15 | P1: Electron-Plasmon interactions in nanostructures
<u>Alexandra Goebel, Lara Román Castellanos, Martik Aghajanian, (Imperial College London)</u> |
| 16:15 | – | 17:00 | P8: First-principles surface photo-chemistry
<u>Thomas Teusch, (University of Oldenburg)</u> |
| 17:00 | – | 17:45 | Postdoc project: Internal screening and dielectric engineering in 2D twisted bilayers
<u>José Pizarro Blanco (University of Bremen)</u> |
| 18:00 | – | 19:30 | Dinner |

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individual	Breakfast
09:00 – 09:45	Guest talk: Ultrafast nanoscale dynamics: a challenge for theory <u>Sascha Schäfer</u> (University of Oldenburg)
09:45 – 10:30	Guest talk: Molecules in Non-Equilibrium Geometries <u>Tim Stauch</u> , (University of Bremen)
10:30 – 11:00	Coffee Break
11:00 – 11:45	P5: Excited carrier dynamics in atomically thin 2D semiconductors <u>Daniel Erben</u> (University of Bremen)
11:45 – 12:30	P6: Influence of defects & environment on photocatalytic properties of TiO ₂ <u>Filippo Balzaretto</u> (University of Bremen)
12:30 – 13:30	Lunch
13:30 – 14:15	Guest talk: Laser-induced charge transfer from real-time TDDFT <u>Prof. Dr. Caterina Cocchi</u> (Humboldt-University Berlin, Germany)
14:15 – 15:00	P7: Energy and charge transfer at surfaces <u>Sayan Maity</u> , Hasan Rahman (Jacobs University Bremen)
15:00 – 15:45	P4: Many-body optics of TMDCs and black phosphorous <u>Frederik Lohof</u> (University of Bremen)
15:45 – 16:15	Coffee Break
16:15 – 17:00	P9: Excited state molecular dynamics using TD-DFT/B in the frequency and time domain <u>Verena Gupta</u> (University of Bremen)
17:00 – 17:45	P10: Electromigration in materials with extended defects <u>Elham Khorasani</u> (University of Bremen)
17:45 – 18:30	Round table I: excited state dynamics and correlations
18:45 – 20:00	Dinner
20:00 – 22:00	Discussions

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individual	Breakfast
09:00 – 09:45	P11 : Electronic structure and charge transport in defective and doped TMDCs <u>Muhammad Sufyan Ramzan</u> (Jacobs University Bremen)
09:45 – 10:30	P12: 2D materials based sensing in liquid solvents Massimo Delle Piane (University of Bremen)
10:30 – 11:00	Coffee Break
11:00 – 11:45	Status Report 1. Kohorte Doktoranden
11:45 – 12:15	New application research topics
12:15 – 13:15	Lunch
13:30 – 15:00	Next steps of RTG: planning of new application
15:00 – 15:30	Departure