

Program of the RTG Retreat
Research Training Group
„Quantum Mechanical Materials Modelling - QM³“
October 30th 9:00 - approx. 14:00

<u>Each project has allocated 10 minutes</u>			
09:00	–	09:10	P1: Electron-Plasmon interactions in nanostructures
09:10	–	09:20	P2: P2: Many-body instabilities in 2D materials
09:20	–	09:30	P3: Many-body approaches to realistic quantum impurity models and Coulomb engineering
09:30	–	09:40	Coffee Break
09:40	–	09:50	P4: Many-body optics of TMDCs and black phosphorous
09:50	–	10:00	P5: Excited carrier dynamics in atomically thin 2D semiconductors
10:00	–	10:10	P6: Influence of defects & environment on photocatalytic properties of TiO ₂
10:10		10:20	Coffee Break
10:20	–	10:30	P7: Energy and charge transfer at surfaces
10:40	–	10:50	P8: First-principles surface photo-chemistry
10:50	–	11:00	P9: Excited state molecular dynamics using TD-DFT/B in the frequency and time domain
11:00		11:10	Coffee Break
11:10	–	11:20	P10: Electromigration in materials with extended defects
11:20	–	11:30	P11: Electronic structure and charge transport in defective and doped TMDCs
11:30	–	11:40	P12: 2D materials based sensing in liquid solvents
11:40		11:50	Coffee Break
11:50	–	12:00	Postdoc project: Internal screening and dielectric engineering in 2D twisted bilayers
12:00	–	12:10	P13: Ultrafast charge transfer and vibronic coupling in TMDC heterostructures
12:10	–	12:20	P14: Electron-phonon coupling across the phase diagram of TMDC-based interfaces
12:20	–	12:30	P15: Distribution of strain between adsorbant and surface in decorated 2d systems
12:30		12:40	Coffee Break
12:40	–	14:00	Group discussion <ul style="list-style-type: none"> • Reelection of the board • Study program: Seminars, colloquia, tutorials, workshops, student corners, key skill qualification courses • Homepage • Review Meeting • Miscellaneous