



Program: 11th DFT Days @ Tübingen 2023

Wednesday, September 20

13.25-13.30 Welcome

Self Assembly

- 13.30-14.00 Jim Lutsko: Using classical DFT to characterize crystallization at the microscopic level
14.00-14.20 Michael Wassermair: Self-assembly phase-behaviour of core-shell particles
14.20-14.50 Roland Roth: Two (almost three) Tales on DFT and the Gyroid

Coffee Break

General Aspects

- 15.20-15.40 Florian Sammüller: Predicting inhomogeneous fluids via machine-learned density functional maps
15.40-16.00 Michael Zimmermann: FMT functionals from one-particle and two-particle cavities: rods on 2D lattices
16.00-16.20 Sophie Hermann: Noether-constrained correlations in equilibrium liquids

Coffee Break

- 16.40-17.10 Andy Archer: Binding potential and wetting behaviour of binary liquid mixtures on surfaces

17.10- **Posters**

Thursday, September 21

Dynamics I

- 9.00-9.30 Salomee Tschopp: Superadiabatic-DDFT under time-dependent external potentials
9.30-10.00 Michael Klatt: When can we uniquely map a classical density to a time-dependent potential?

Coffee Break

- 10.30-11.00 Michael te Vrugt: Passive and active field theories for disease spreading
11.00-11.30 Matthias Fuchs: Hard Spheres going backwards in time differently

Lunch Break

Molecules / Anisotropic Particles

- 13.30-14.00 Luc Belloni: WDA approach applied to Molecular DFT for CO₂ and H₂O systems
14.00-14.30 Antoine Carof: Molecular DFT and HNC for supercritical fluids
14.30-14.50 Anouar el Moumane: Biaxial nematic order in Fundamental Measure Theory

Coffee Break

Charges

- 15.20-15.50 Dirk Gillespie: Creating charge inversion in 1:1 electrolytes by changing the energetics balance via the dielectric constant
15.50-16.20 Daniel Borgis: Dipolar saturation in water (revisited with DFT)

Coffee Break

- 16.50-17.20 Guillaume Jeanmairet: Electron transfer of functionalized quinones
17.20-17.40 Helene Berthoumieux: Electrolytes at the nanoscale : a field theory description

19.00- Conference Dinner

Friday, September 22

Dynamics II

- 9.00-9.30 Daniel de las Heras: Machine learning the functional mapping of power functional theory
9.30-10.00 Rene Wittmann: Mechano-response in growing bacterial colonies: cell-size distributions from DDFT
10.00-10.20 Debankur Das: Memory induced Magnus effect

Coffee Break

- 10.50-11.20 Carmine Anzivino: Microscopic theory for the shear-induced structure distortion in concentrated suspensions of spherical colloids
11.20-11.50 Matthias Krüger: Painted particle model for mobility in mixtures and its consequences in dynamical (density functional) theory
11.50-12.00 Closing remarks

Posters

Mohamed Houssein:	Molecular density functional theory of solvation for supercritical CO ₂
Silas Robitschko:	Local force fluctuations in inhomogeneous liquids
Jonas Köglmayr:	Drag forces in inhomogeneous counterdriven binary mixtures
Nico Stuhlmüller:	Local measures of fluctuations in inhomogeneous liquids
Maxime Labat:	Computing Redox properties in solution with QM/MDFT
Alessandro Simon:	A density functional for patchy particles from machine learning