

Final Program 10th DFT days, Sep 26-28, 2022

Mon Sep 26			
	13.25-13.30	Welcome	
		General Aspects	
	13.30-14.00	Roland Roth	In Search for a Second Critical Point
	14.00-14.30	Andy Parry	Wetting Transitions: Things I didn't know
	14.30-14.50	Alessandro Simon	A density functional for patchy particles from Machine Learning
		Coffee Break	
	15.20-15.40	Salomé Tschopp	Inhomogeneous density profiles from the virial route
	15.40-16.10	Joe Brader	First-principles superadiabatic theory for the dynamics of inhomogeneous fluids
		Coffee Break	
	16.40-17.10	Uwe Thiele	On the relation of the Maxwell construction for phase transitions and bifurcation diagrams
	17.10-17.40	Matthias Schmidt	What is Liquid, from Noether's Perspective?
	18.00-	Posters	(with drinks)
		Dynamics	
Tue Sep 27	9.00-9.30	Jim Lutsko	Reconsidering Power Functional Theory
	9.30-10.00	Michael te Vrugt	Derivation and analysis of a phase field crystal model for a mixture of active and passive particles
	10.00-10.20	Jonna Roden	PDE-constrained optimization for multiscale particle dynamics
		Coffee Break	
	10.50-11.20	Ben Goddard	DDFT for Opinion Dynamics
	11.20-11.50	Andy Archer	Stochastic transitions: Paths over higher energy barriers can dominate in the early stages
		Lunch Break	
		Electrostatics	
	14.00-14.30	Peter Cats	In-plane structure of electric double layers
	14.30-15.00	Andreas Härtel	CapDFT - C++ support for DFT implementations/ Differential capacitances in models and experiments
	15.00-15.30	Dirk Gillespie	Charged systems: Turns out we knew even less than we thought
		Coffee Break	
	16.00-16.30	Daniel Borgis	Nonlocal electrostatics in confined conditions: insights from cDFT
	16.30-17.00	Guillaume Jeanmairet	Modeling aqueous electrolyte with Molecular Density Functional Theory
		Coffee Break	
		Applications	
	17.30-18.00	Daniel de las Heras	Sedimentation path theory for mass-polydisperse colloidal systems
	18.00-18.20	Florian Sammüller	Inhomogeneously sheared colloidal gels
	19.00-	Conference Dinner	(Ludwigs)
Wed Sep 28		Crystals	
	9.00-9.30	Matthias Fuchs	Thermomechanics of complex crystals: From DFT and projection-operators to transport laws of continuum mechanics
	9.30-9.50	Cedric Schoonen	Surface tension-induced crystal polymorphism
	9.50-10.10	Saswati Ganguly	Statistical Mechanics of yielding in ordered solids
		Coffee Break	
		Solvation and Confinement	
	10.40-11.10	Bob Evans	Determining Solvent Mediated Interactions: what has DFT contributed?
	11.10-11.40	Antoine Carof	Ultrafast calculation of solvation in supercritical CO2 with classical DFT
	11.40-12.10	Rene Wittmann	DFT and confinement - from topological defects to statistics of particle uptake
	12.10-12.15	Closing remarks	