Program, NSF/CECAM summer school 2017

	Mon, July 17	Tue, July 18	Wed, July 19	Thu, July 20	Fri, July 21	Sat, July 22	Mon, July 24	Tue, July 25	Wed, July 26	Thu, July 27
9:00-9:30		Andreas Görling – basic DFT concepts, applications	Alexandre Tkatchenko – DFT and dispersion interactions	HT Mertig	Kristen Fichthorn - An introduction to rare-event dynamics	Michele Ceriotti – advanced molecular dynamics	Lasse Jensen – enhanced Raman spectroscopy	Gabor Csanyi – The GAP potential	Stefano Piana – Large-Scale Molecular Dynamics Simulations: Force-Field	HT Crespi
9:30-10:00				HT Tkatchenko						HT Kaxiras
10:00-10:30		Claudia Draxl – time-dependent DFT	Francesco Sottile - time-dependent DFT	Michael Janik – electro-chemistry	Elisa Molinari – excitons	HT Dabo	Kristen Fichthorn – (Superbasin) Kinetic Monte Carlo	Luca Ghiringhelli - configurational sampling	Tim Kaxiras – Machine Learning	HT Curtarolo *Closing remarks*
10:30-11:00						HT Janik				
11:00-11:30		break	break	break	Break	break	Break	Break	break	
11:30-12:00		Silke Biermann – dynamic mean-field theory and strongly correlated systems	Ingrid Mertig – topological insulators	Stefano Baroni – density functional perturbation theory	Philippe Sautet – catalysis	HT Catlow	HT Yakobson	Jim Pfaendtner– configurational sampling of biomolecules	HT Ghiringhelli	
12:00-12:30						HT Ceriotti	HT Jensen		HT Pfaendtner	
12:30-14:30		Lunch Break	Lunch Break	Lunch Break	Lunch Break / Boris Yakobson – 2D Materials		Lunch Break	Lunch Break	Lunch Break	
14:30-15:00	Welcome by the organizers	Michael Seidl – electronic structure theory of strongly correlated systems	HT Görling	HT Sottile	HT Molinari		Karsten Reuter – multi-scale modelling of catalysis	HT Reuter	Stefano Curtarolo – high-throughput calculations	
15:00-15:30	Matthias Scheffler – electronic-structure theory (introduction)		HT Biermann	Ismaila Dabo – DFT functionals	HT Baroni			HT Sinnott		
15:30-16:00		HT Draxl	HT Seidl		HT Sautet		HT Fichthorn	HT Csanyi	HT Piana	
16:00-16:30	Kristen Fichthorn – sample that: DFT in multi-scale materials simulation	break	break	break	break		Break	break	Break	
16:30-17:00		*Poster Parade*	*Poster Session*	*Poster Session*	C. Richard A. Catlow – embedding techniques		Susan B. Sinnott – the COMB potential	Matthias Scheffler – NOMAD	Vin Crespi- Choosing the Best Research Problems	
17:00-17:30	*Reception*									
17:30-18:00									↓ Conference Dinner at 7 pm	

There will be an excursion on Sunday, July 23, 2017 and a conference dinner

HT: hot topic talk

as of 21.7.2017