MONDAY 25 September 2017		TUESDAY 26 September 2017		WEDNESDAY 27 September 2017	
		9:00 - 10:00	Ward	9:00 - 10:00	Todorovic
		10:00 - 10:30	Mali	10:00 - 10:30	Scherbela
		10:30 - 11:00	Balzer	10:30 - 11:00	Breuer
			coffee break		coffee break
		11:30 - 12:30	Tkatchenko	11:30 - 12:30	Myerson
		12:30 - 13:00	Poster	12:30 - 13:00	Chattopadhyay
			lunch		CONCLUSION
12:45 - 13:00	WELCOME	13:00 - 14:30	Poster		
13:00 - 14:00	Griesser	14:30 - 15:30	Forker		
14:00 - 15:00	Loo	15:30 - 16:00	Roese	15:00	excursion
15:00 - 15:30	Gbabode	16:00 - 16:30	Th. Wagner		
	coffee break	16:30 - 17:00	Matkovic		
16:00 - 17:00	Ocko		coffee break		
17:00 - 17:30	Smilgies	17:30 - 18:30	Sugden		
17:30 - 18:00	Schiek	18:30 - 19:00	Rozboril		Invited talk
18:00 - 18:30	Rivalta				Contributed talk
		20:00	dinner		Poster

Program of the Workshop

Monday
25th September 2017

12:45 – 13:00	Welcome

SESSION 1:
Chairman: A. Daniel Boese, Graz University

13:00 – 14:00	**Ulrich Griesser** (University of Innsbruck, Austria) Pathways to polymorphs in molecular crystals
14:00 – 15:00	**Lynn Loo** (Princeton University, NJ, USA) Polymorphic accessibility and stability in molecular semiconductor thin films
15:00 – 15:30	**Gabin Gbabode** (Normandie University, Rouen, France) Preliminary results on the polymorphic behavior in thin films of a small organic model molecule: n-methylurea
15:30 – 16:00	**Coffee Break**

SESSION 2:
Chairman: Oliver Werzer, Graz University

16:00 – 17:00	**Ben Ocko** (Brookhaven National Laboratory, NY, USA) Surface feezing
17:00 – 17:30	**Detlef-M. Smilgies** (Cornell University, NY, USA) Transient polymorphs during processing of organic semiconductors
17:30 – 18:00	**Manuela Schiek** (University of Oldenburg, Germany) Polymorphic phases of an aniline-squaraine in spin casted and vapor deposited thin films
18:00 – 18:30	**Ariana Rivalta** (University of Bologna, Italy) Polymorphs and Surface Induced Structures in drug thin films investigated by Raman spectroscopy

Tuesday
26th September 2017

SESSION 3:
Chairman: Oliver Hofmann, Graz University of Technology

9:00 – 10:00	**Michael D. Ward** (New York University, NY, USA) The role of epitaxy and confined interfaces in thin film and crystal polymorphism
10:00 – 10:30	**Kunal S. Mali** (Leuven Chem and Tech, Belgium) Surface-supported multicomponent supramolecular architechture: interactions and stimulus responsive behaviour
10:30 – 11:00	**Frank Balzer** (South Danish University, Sonderborg, Denmark) Formation and electrostatic surface potential of functionalized quarter-phenylene nanofibers
11:00 – 11:30	**Coffee Break**

SESSION 4:
Chairman: Oliver Hofmann, Graz University of Technology

11:30 – 12:30	**Alexandre Tkatchenko** (University of Luxembourg, Luxembourg) First-principles modeling of molecular polymorphism in crystals and on surfaces
12:30 – 14:30	**Poster Session including Lunch**

SESSION 5:
Chairman: Andrew O. F. Jones, Anton Paar, Graz

14:30 – 15:30	**Roman Forker** (Friedrich Schiller University Jena, Germany) Physisorbed molecular adlayer exhibiting temperature- and coverage-dependent polymorphism
15:30 – 16:00	**Peter Roese** (Technische Universität Dortmund, Germany) XPS/XPD measurements of self-assembled caffeine monolayers on Ag(110)
16:00 – 16:30	**Thorsten Wagner** (Jophannes Kepler Univerisity Linz, Austria) The growth of α – sexithiophene on different silver surfaces
16:30 – 17:00	**Aleksandar Matković** (Montanuniversität Leoben, Austria) Contact planes of small rod-like molecules on graphene and hexagonal boron nitride
17:00 – 17:30	**Coffee Break**

SESSION 6:
Chairman: Andrew O. F. Jones, Anton Paar, Graz

17:30 – 18:30	**Isaac Sudgen** (Imperial College London, UK) Recent advances in *ab initio* crystal structure prediction
18:30 – 19:00	**Jakub Rozbořil** (Masaryk University, Brno, Czech Republic) In-situ X-ray diffraction annealing study on an anthradithiophene derivative
20:00	**Workshop dinner "Meerscheinschlössl"**

Wednesday
27th September 2017

SESSION 7:
Chairman: Roland Resel, Graz University of Technology

9:00 – 10:00	**Milica Todorović** (Aalto University, Finland) Efficient Bayesian inference of surface adsorption
10:00 – 10:30	**Michael Scherbela** (Graz University of Technology, Austria) Computational polymorph prediction for organic/inorganic interfaces using machine learning
10:30 – 11:00	**Tobias Breuer** (Philipps-University Marburg, Germany) Influence of surface roughness on polymorph formation in organic thin films
11:00 – 11:30	**Coffee Break**

SESSION 8:
Chairman: Roland Resel, Graz University of Technology

11:30 – 12:30	**Allan S. Myerson** (Massachusetts Institute of Technology, MA, USA) Nucleation of organic molecular crystals on surfaces and in nanopores
12:30 – 13:00	**Basab Chattopadhyay** (Université Libre de Bruxelles, Belgium) A thermal gradient approach towards polymorph selection
15:00 –	**Excursion**

Posters

(1) Selective, temperature-induced F4TCNQ desorption from p-doped P3HT films
H. Hase, A. Opitz, N. Koch, I. Salzmann

(2) Epitaxially ordered Metal-Organic-Frameworks based on copper-benzenedioic acid
S. Hofer, A. Jones, R. Resel, K. Okada, R. Ricco, P. Falcaro

(3) First-principles molecular crystal structure prediction: The importance of collective van der Waals interactions and free energies
J. Hoja, H.-Yu Ko, R. Car, R. A. DiStasio Jr., A. Tkatchenko

(4) Computational phase diagram prediction for organic monolayers on metal substrates
L. Hörmann, M. Scherbela, V. Obersteiner, O.T. Hofmann

(5) Photochemical switching of azobenzene derivatives on an insulating surface
S. Jaekel, A. Richter. R. Lindner, R. Bechstein, A. Kühnle, St. Hecht, L. Grill

(6) Understanding polymorph selection in nabumentone thin films at surfaces
M. Kaltenegger, O. Werzer, Ch. Röthel

(7) Biaxial oriented growth of pentacene on rippled glass surfaces
S. Pachmajer, O. Werzer, A. Perrotta, R. Resel

(8) Appearance of a surface induced crystal structure of 6,6'-dibromoindigo
M. Truger, C. Röthel, D. Kriegner, I. Salzmann, J. Simbrunner, R. Resel

(9) Complex behaviour of caffeine crystallites on solid surfaces
C. Röthel, M. Radziown, C. Simbrunner, R. Resel, O. Werzer

(10) The substrate-induced phase of C_8O-BTBT-OC_8 detected by mid-infrared and lattice phonon Raman spectroscopy
B. Schrode, A.O.F. Jones, R. Resel, R. Schennach, A. Brillante, T. Salzillo, E. Venuti

(11) Photoluminescence as a probe of molecular organization in PDI8-CN2 ultra-thin films
A. Brillante, T. Salzillo, R.G. Della Valle, E. Venuti, F. Borgatti, E. Lunedei, F. Liscio, S. Milita, C. Albonetti

(12) Accurate calculations of molecular crystals
O. A. Loboda, G. A. Dolgonos, A. D. Boese

(13) Addressing conformational and vibrational entropy in bio-organic systems
M. Rossi, D. Makismov, C. Baldauf

(14) *In-situ* crystallization and gel formation of thermodynamically unstable polymorphs: a SWAXS study of caffeine in isopropanol
A. O. F. Jones, H. M. A. Ehmann, A. Keilbach, A. Moser, C. Röthel, O. Werzer

(15) A fast alternative to periodic DFT calculations: DFT embedded into DFTB
G. A. Dolgonos, O. A. Loboda, A. D. Boese