

## EXTMOS Erice School programme

### Monday 1 Oct arrivals

### Tuesday 2 Oct

9.15-9.30		C. Zannoni, UNIBO, ISLC	Welcome
9.30-10.20	L1	A. Walker, U. Bath	100% Organic: Understanding Organic Electronics from Molecules to Devices
10.20-11.10	L2	W. Wenzel, KIT	Multiscale Modelling of Nanoscale Materials and Electronic Transport
11.10-11.30	CB		Coffee Break
11.30-12.20	L3	F. Ortmann, T. U. Dresden	Ab Initio-Based Approach to the Density of States of Doped Organic Semiconductors
12.20-15.00	LB		Lunch Break
15.00-15.50	L4	C. Zannoni, UNIBO	Modelling Morphologies by Molecular Dynamics
15.50-16.40	L5	G. Schweicher, U. Cambridge	OFET and Charge Transport in Small Molecule Organic Semiconductors
16.40-17.00	CB		Coffee Break
17.00-17.50	L6	J. Gierschner, Madrid IAS	Organic Solid State Emitters by Design 1/2
17.50-18.40	L7	P. Bobbert, T. U. Eindhoven	Molecular-Scale Modeling of Charge Transport and Excitonics in Organic Devices 1/2

### Wednesday 3 Oct

9.00-9.50	L8	F. Ortmann, T. U. Dresden	Theoretical Prediction of the Density of States of n-Doped Organic Films and Comparison to Experiments
9.50-10.40	L9	I. Duchemin, CEA Grenoble	Electronic and Optical Properties of Organic Systems with Embedded Many-Body Perturbation Theory
10.40-11.00	CB		Coffee Break
11.00-11.50	L10	O. M. Roscioni, L. Querciagrossa, M. Ricci, UNIBO	Atomistic and Coarse-Grained Modelling and Simulations
11.50-12.40	L11	P. Friederich KIT	Design Principles for Charge Carrier Mobility and Anisotropic Orientation of Organic Semiconductors
12.40-15.00	LB		Lunch Break
15.00-15.50	L12	G.A.H. Wetzelaer, MPG Mainz	Injection, Transport, and Recombination of Charges in Organic-Semiconductor Diodes 1/2
15.50-16.40	L13	T. Deutsch, CEA Grenoble	Applications of Wavelet-Based Density Functional Theory
16.40-17.00	CB		Coffee Break
17.00-17.50	L14	P. Bobbert, T. U. Eindhoven	Molecular-Scale Modeling of Charge Transport and Excitonics in Organic Devices 2/2
17.50-18.40	L15	A. Smith, U. Bath	Simulating Organic Semiconductors: the Challenge of Amorphous Materials

**Thursday 4 Oct**

9.00-9.50	L16	I. Thompson, U. Bath	Modelling Charge Transport in Organic Semiconductors at the Mesoscale
9.50-10.40	L17	D. Beljonne, U. Mons	Charge Transport in Carbon-Based Materials: A Microscopic View
10.40-11.00	CB		Coffee Break
11.00-11.50	L18	Y. Olivier, U. Mons	Dissecting the Nature of the Relevant Singlet and Triplet Excited States in TADF Molecular Materials
11.50-12.20	O1	G. Londi, U. Mons	Efficient Exciton Diffusion in a Donor-Acceptor Conjugated Dye for Solar Cells Applications: Theoretical Insights
12.20-14.30	LB		Lunch Break
14.30-19.30	EX		Excursion (Segesta Archeological site)

**Friday 5 Oct**

9.00-9.50	L10	B. Yaglioglu, FlexEnable	FlexEnable's Organic Thin Film Transistor Technology and its Applications
9.50-10.40	L20	G.A.H. Wetzelaer, MPG Mainz	Injection, Transport, and Recombination of Charges in Organic-Semiconductor Diodes 2/2
10.40-11.00	CB		Coffee Break
11.00-11.50	L21	C. Rolin, IMEC	Impact of Contact Resistance on the Integration of Organic Thin Film Transistors
11.50-12.40	L22	T. Neumann, Nanomatch	Performing Multiscale OLED Simulations Using Industry-Ready Software
12.40-15.00	LB		Lunch Break
15.00-16.40	L23 L24	T. Neumann, Nanomatch	Demo (Nanomatch)
16.40-17.00	CB		Coffee Break
17.00-18.40	PS		<i>EXTMOS technical meeting (only for EXTMOS partners)</i>
20.00-	SD		Social Dinner

**Saturday 6 Oct**

9.00-9.50	L25	G. Schweicher, U. Cambridge	Structure-Property Relationships in Thienacenes for Improved Charge Transport
9.50-10.40	L26	A. Fedai, KIT	Doping-Induced Phenomena in Organic Semiconductors: Insights from kMC Simulations
10.40-11.00	CB		Coffee Break
11.00-11.50	L27	J. Gierschner, Madrid IAS	Organic Solid State Emitters by Design 2/2
11.50-12.40	L28	A. Nejim, Silvaco	Device Level Design for the Microelectronic Industry
12.40-15.00	LB		Lunch Break
15.00-16.40	L29 L30	A. Nejim, Silvaco	Demo (Silvaco)
16.40-17.00	CB		Coffee Break
17.00-17.50	L31	A. Walker, U. Bath	Conclusions and Perspectives