nanoGe Fall Meeting 2018 (FallMeeting18)

S8 Modelling Perovskite Solar Cells from the Microscale to the Macroscale

Torremolinos, Spain, 2018 October 22nd - 23rd
Conference Chairs: Alison Walker and Claudio Quarti

Conference Program

October 22nd - Day 1 (Monday)	
	Plenary session 1 Chair: Mischa Bonn
09:00 - 09:30 1-K1	Victor Klimov *(Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA)* Colloidal Quantum Dot Lasing: Historical Perspective and Recent Progress
	Plenary Session 2 Chair: Kevin Sivula
09:00 - 09:30 2-K1	Yun Jeong Hwang *(Korea Institute of Science and Technology (KIST))*, Byoun Koun Min, Hyeong-Suk Oh Electrochemical Conversion of CO2 toward Valuable Chemicals for Solar-to-Chemical Conversion Application
	PerMod S8.1 Chair: Alessio Gagliardi
09:30 - 10:00 S8.1-I1	Beat Ruhstaller *(Zurich Univ. of Appl. Sciences (ZHAW), Inst. of Computational Physics)*, Evelyne Knapp, Martin Neukom, Andreas Schiller, Stéphane Altazin Electronic, Ionic and Optical Perovskite Solar Cell Modeling and Experimental Validation
10:00 - 10:30 S8.1-I2	Juan A. Anta *(Área de Química Física, Universidad Pablo de Olavide, E-41013 Sevilla, Spain)* Modeling and Interpretation of Small Perturbation Measurements in Perovskite Solar Cells
10:30 - 11:00	**Coffee Break**
	PerMod S8.2 Chair: Amanda Neukirch
11:00 - 11:30 S8.2-O3	Uli Würfel *(Fraunhofer Institute for Solar Energy Systems (ISE), Heidenhofstraße 2, 79110 Freiburg, Germany)*, Moritz Unmüssig Why Do Perovskite Solar Cells that Have a Reduced Open-Circuit Voltage due to Surface Recombination Not Show Hysteresis?
11:30 - 12:00 S8.2-O1	Marten Koopmans *(Photophysics and OptoElectronics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, The Netherlands)*, Jan Anton Koster A comprehensive numerical study of the implications of s-shaped JV characteristics in perovskite solar cells
12:00 - 12:30 S8.2-O2	Nadège Marchal *(University of Mons (UMONS), Laboratory for Chemistry of Novel Materials, Center for Innovation and Research in Materials and Polymers (CIRMAP), Mons (Belgium))*, Claudio Quarti, David Beljonne Effect of Electronically Inert Organic Spacers on the Optoelectronic Properties of 2D Hybrid Perovskites
12:30 - 14:30	**Lunch**
	PerMod S8.3 Chair: Edoardo Mosconi
14:30 - 15:00	
15:00 - 15:30 S8.3-I1	Amanda Neukirch *(Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States)*, Jacky Even, Claudine Katan, Sergei Tretiak Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Replacement in Halide Perovskites

15:30 - 16:00 S8.3-O1	Juan Bisquert *(Institute of Advanced Materials (INAM), UniversitatJaume I, 12006 Castelló, Spain)*, Agustín Bou, Sandheep Ravishankar Theory of Frequency Perturbation Techniques for Perovskite Solar Cells
16:00 - 16:30 S8.3-O2	Matthew Wolf *(Department of Physics, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom)*, Lewis Irvine, Ian Thompson, Alison Walker Meso-Scale Modelling of Charge Transport in Halide Perovskites
16:30 - 17:00 S8.3-O3	Vanessa Wood *(ETH Zurich, Department of Information Technology and Electrical Engineering)* Vibrations and Electron-Phonon Coupling in Lead Halide Perovskite Nanocrystals
October 23rd - Day 2 (Tuesday)	
	PerMod S8.4 Chair: Beat Ruhstaller
09:00 - 09:30 S8.4-I1	Giles Richardson *(University of Southampton)* How Transport Layer Properties affect Perovskite Solar Cell Performance: Insights from a Coupled Charge Transport/ion Migration Model
09:30 - 10:00 S8.4-I2	Alessio Gagliardi *(Technische Universität München)* Simulation of Perovskite Solar Cells: the Role of Internal Interfaces
10:00 - 10:30 S8.4-O1	Daniele Meggiolaro *(D3-Computation, Istituto Italiano di Tecnologia)*, Edoardo Mosconi, Filippo De Angelis Defects in Lead Halide Perovskites: a Computational Perspective
10:30 - 11:00	**Coffee Break**
	PerMod S8.5 Chair: Juan A. Anta
11:00 - 11:30 S8.5-O1	Vincent Le Corre *(Photophysics and OptoElectronics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, The Netherlands)*, Lorena Perdigón Toro, Markus Feuerstein, Martin Stolterfoht, Dieter Neher, L. Jan Anton Koster Transport Layers Limit the Efficiency of Perovskite Solar Cells: an Experimental and Theoretical Study.
11:30 - 12:00 S8.5-O2	Manuel García-Rosell *(Departamento de Electrónica y Tecnología de Computadores, CITIC-UGR, Universidad de Granada, 18071 Granada, Spain)*, Agustín Bou, Juan A. Jiménez-Tejada, Juan Bisquert, Pilar Lopez-Varo Influence of Ion Migration on the performance of the Selective Contact Heterojunctions in Perovskite Solar Cells
12:00 - 12:30 S8.5-O3	Juan Jesus Gallardo *(University of Cádiz)*, Javier Navas, Fran Reyes-Perez, Teresa Aguilar, Rodrigo Alcántara, Concha Fernández-Lorenzo CsSnBr3, a Lead-Free Perovskite with Photocatalytic Activity
12:30 - 14:30	**Lunch**
	joint session S7/S8
14:30 - 15:00 S7/S8-I1	Filippo De Angelis *(Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Perugia, Italy)* Defect photophysics of metal-halide pero
15:00 - 15:30 S7/S8-I2	Koichi Yamashita *(Department of Chemical System Engineering, Graduate School of Engineering, The University of Tokyo)* Charge Separation and Charge Carrier Trapping of Lead Iodide Perovskites
15:30 - 16:00 S7/S8-I3	Edoardo Mosconi *(Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto CNR di ScienzeTecnologie Molecolari (ISTM-CNR), Via Elce di Sotto 8, 06123, Perugia, Italy.)* Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics
16:00 - 16:30 S7/S8-I4	Claudine Katan *(Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR6226, F-35000 RENNES)*, Boubacar Traore, Mikaël Képénékian, Laurent Pedesseau, Jean-Christophe Blancon, Wanyi Nie, Hsinhan Tsai, Sergei Tretiak, Constantinos Stoumpos, Mercouri Kanatzidis, Aditya Mohite, Jacky Even Halide Perovskites: Recent Advances in Optoelectronic Properties from Atomic Scale Modelling

	PerMod S8.6
16:30 - 17:00 S8.6-I1	Ursula Roethlisberger *(Swiss Federal Institute of Technology, EPFL, ISIC, LCBC, CH-1015, Lausanne, Switzerland)*, Paramvir Ahlawat, Michele Parrinello Modelling Nucleation and Growth of Lead Halide Perovskites
17:30 - 19:00	**Poster Session**

Poster Contribution

290	Azimatu Seidu *(Department of Applied Physics, Aalto University School of Science)*, Lauri Himanen Coating Hybrid Perovskites: A Database-Driven Study
316	Elnaz Ghahremanirad, Agustín Bou *(Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castelló, Spain)*, Saeed Olyaee, Juan Bisquert Inductive Loop in the Impedance Response of Perovskite Solar Cells Explained by Surface Polarization Model