

nanoGe Fall Meeting 2018 (FallMeeting18)

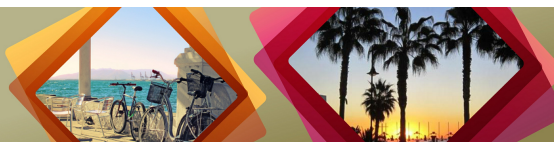
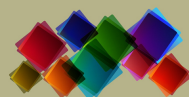
S8 Modelling Perovskite Solar Cells from the Microscale to the Macroscale

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	<u>Victor Klimov</u> (<i>Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA</i>) Colloidal Quantum Dot Lasing: Historical Perspective and Recent Progress
Plenary Session 2 Chair: Kevin Sivula	
09:00 - 09:30 2-K1	<u>Yun Jeong Hwang</u> (<i>Korea Institute of Science and Technology (KIST)</i>), Byoun Koun Min, Hyeong-Suk Oh Electrochemical Conversion of CO ₂ toward Valuable Chemicals for Solar-to-Chemical Conversion Application
PerMod S8.1 Chair: Alessio Gagliardi	
09:30 - 10:00 S8.1-11	<u>Beat Ruhstaller</u> (<i>Zurich Univ. of Appl. Sciences (ZHAW), Inst. of Computational Physics</i>), Evelyne Knapp, Martin Neukom, Andreas Schiller, Stéphane Altazin Electronic, Ionic and Optical Perovskite Solar Cell Modeling and Experimental Validation
10:00 - 10:30 S8.1-12	<u>Juan A. Anta</u> (<i>Área de Química Física, Universidad Pablo de Olavide, E-41013 Sevilla, Spain</i>) 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	<u>Uli Würfel</u> (<i>Fraunhofer Institute for Solar Energy Systems (ISE), Heidenhofstraße 2, 79110 Freiburg, Germany</i>), 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	<u>Marten Koopmans</u> (<i>Photophysics and Optoelectronics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, The Netherlands</i>), 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	<u>Nadège Marchal</u> (<i>University of Mons (UMONS), Laboratory for Chemistry of Novel Materials, Center for Innovation and Research in Materials and Polymers (CIRMAP), Mons (Belgium)</i>), 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 S8.3-11	<u>Saiful Islam</u> (<i>Department of Chemistry, University of Bath</i>) Structural Distortion and Molecular Cation Dynamics in Mixed-Cation Perovskites
15:00 - 15:30 S8.3-12	<u>Amanda Neukirch</u> (<i>Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States</i>), Jacky Even, Claudine Katan, Sergei Tretiak Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Replacement in Halide Perovskites



- 15:30 - 16:00 Juan Bisquert (*Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castelló, Spain*), Agustín Bou,
S8.3-O1 Sandheep Ravishankar
Theory of Frequency Perturbation Techniques for Perovskite Solar Cells
- 16:00 - 16:30 Matthew Wolf (*Department of Physics, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom*),
S8.3-O2 Lewis Irvine, Ian Thompson, Alison Walker
Meso-Scale Modelling of Charge Transport in Halide Perovskites
- 16:30 - 17:00 Vanessa Wood (*ETH Zurich, Department of Information Technology and Electrical Engineering*)
S8.3-O3 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 Giles Richardson (*University of Southampton*)
S8.4-I1 How Transport Layer Properties affect Perovskite Solar Cell Performance: Insights from a Coupled Charge
Transport/ion Migration Model
- 09:30 - 10:00 Alessio Gagliardi (*Technische Universität München*)
S8.4-I2 Simulation of Perovskite Solar Cells: the Role of Internal Interfaces
- 10:00 - 10:30 Daniele Meggiolaro (*D3-Computation, Istituto Italiano di Tecnologia*), Edoardo Mosconi, Filippo De Angelis
S8.4-O1 Defects in Lead Halide Perovskites: a Computational Perspective

10:30 - 11:00 **Coffee Break**

PerMod S8.5

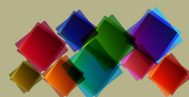
Chair: Juan A. Anta

- 11:00 - 11:30 Vincent Le Corre (*Photophysics and OptoElectronics, Zernike Institute for Advanced Materials, University of
S8.5-O1 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 Manuel García-Rosell (*Departamento de Electrónica y Tecnología de Computadores, CITIC-UGR, Universidad
S8.5-O2 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 Juan Jesus Gallardo (*University of Cádiz*), Javier Navas, Fran Reyes-Perez, Teresa Aguilar, Rodrigo Alcántara,
S8.5-O3 Concha Fernández-Lorenzo
CsSnBr₃, a Lead-Free Perovskite with Photocatalytic Activity

12:30 - 14:30 **Lunch**

joint session S7/S8

- 14:30 - 15:00 Filippo De Angelis (*Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Perugia,
S7/S8-I1 Italy*)
Defect photophysics of metal-halide pero
- 15:00 - 15:30 Koichi Yamashita (*Department of Chemical System Engineering, Graduate School of Engineering, The
S7/S8-I2 University of Tokyo*)
Charge Separation and Charge Carrier Trapping of Lead Iodide Perovskites
- 15:30 - 16:00 Edoardo Mosconi (*Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto CNR di
S7/S8-I3 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 Claudine Katan (*Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de
S7/S8-I4 Rennes) - UMR6226, F-35000 RENNES*), Boubacar Traore, Mikael 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 Olyaei, Juan Bisquert
Inductive Loop in the Impedance Response of Perovskite Solar Cells Explained by Surface Polarization Model