

## nanoGe Fall Meeting 2018 (FallMeeting18)

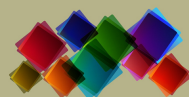
### S8 Modelling Perovskite Solar Cells from the Microscale to the Macroscale

Torremolinos, Spain, 2018 October 22nd - 23rd

Conference Chairs: Alison Walker and Claudio Quarti

### Conference Program

October 22nd - Day 1 (Monday)	
	<p><b>Plenary session 1</b> Chair: Mischa Bonn Room: Mediterraneo ABC</p>
09:00 - 09:30 1-K1	<p><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</p>
	<p><b>Plenary Session 2</b> Chair: Kevin Sivula Room: Torremolinos AB</p>
09:00 - 09:30 2-K1	<p><u>Yun Jeong Hwang</u> (<i>Korea Institute of Science and Technology (KIST)</i>), Byoun Koun Min, Hyeong-Suk Oh Electrochemical Conversion of CO<sub>2</sub> toward Valuable Chemicals for Solar-to-Chemical Conversion Application</p>
	<p><b>PerMod S8.1</b> Chair: Alessio Gagliardi Room: Torremolinos C</p>
09:30 - 10:00 S8.1-11	<p><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</p>
10:00 - 10:30 S8.1-12	<p><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</p>
10:30 - 11:00	<p><b>Coffee Break</b></p>
	<p><b>PerMod S8.2</b> Chair: Amanda Neukirch Room: Torremolinos C</p>
11:00 - 11:30 S8.2-O3	<p><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?</p>
11:30 - 12:00 S8.2-O1	<p><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</p>
12:00 - 12:30 S8.2-O2	<p><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</p>
12:30 - 14:30	<p><b>Lunch</b></p>
	<p><b>PerMod S8.3</b> Chair: Edoardo Mosconi Room: Torremolinos C</p>
14:30 - 14:45 S8.3-O4	<p>Elnaz Ghahremanirad, <u>Agustín Bou</u> (<i>Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castelló, Spain</i>), Saeed Olyaei, Juan Bisquert Inductive Loop in the Impedance Response of Perovskite Solar Cells Explained by Surface Polarization Model</p>



# nanoGe Fall Meeting

Torremolinos-Spain

October 22-26, 2018



nanoGe

- 14:45 - 15:00 Azimatu Seidu (*Department of Applied Physics, Aalto University, P.O.Box 11100, FI-00076 Aalto, Finland*), Lauri S8.3-O5  
Himanen, Jingrui Li, Patrick Rinke  
Database-driven study for hybrid perovskite coating materials
- 15:00 - 15:30 Amanda Neukirch (*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States*), Jacky S8.3-I1  
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), UniversitatJaume 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  
Room: Torremolinos C

- 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  
Room: Torremolinos C

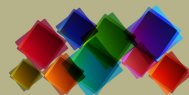
- 11:00 - 11:30 Vincent Le Corre (*Photophysics and OptoElectronics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, The Netherlands*), Lorena Perdigón Toro, Markus Feuerstein, Martin S8.5-O1  
Stolterfoht, Dieter Neher, L. Jan Anton Koster  
Transport Layers 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 de Granada, 18071 Granada, Spain*), Agustín Bou, Juan A. Jiménez-Tejada, Juan Bisquert, Pilar Lopez-Varo S8.5-O2  
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  
CsSnBr<sub>3</sub>, a Lead-Free Perovskite with Photocatalytic Activity

### 12:30 - 14:30 Lunch

### joint session S7/S8

Room: Torremolinos DE

- 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 Scienze e Tecnologie Molecolari (ISTM-CNR), Via Elce di Sotto 8, 06123, Perugia, Italy.*), García Espejo García Espejo, Filippo De Angelis  
S7/S8-13

First Principles Modeling of Mixed 2D/3D Organohalide Perovskites

16:00 - 16:30 **Claudine Katan** (*Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de 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  
S7/S8-14

Halide Perovskites: Recent Advances in Optoelectronic Properties from Atomic Scale Modelling

### **PerMod S8.6**

Chair: Claudio Quarti

Room: Torremolinos C

16:30 - 17:00 **Ursula Roethlisberger** (*Swiss Federal Institute of Technology, EPFL, ISIC, LCBC, CH-1015, Lausanne, Switzerland*), Paramvir Ahlawat, Michele Parrinello  
S8.6-11

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