

nanoGe Fall Meeting19 (NGFM19)

#PERFuDe19. Halide perovskites: when theory meets experiment from fundamentals to devices

Berlin, Germany, 2019 November 6th - 8th

Conference Chairs: Claudine Katan, Wolfgang Tress and Simone Meloni

Conference Program

November 6th - Day 4 (Wednesday)	
	Plenary Session Chair: Jacky Even 09:00 - 09:30 <u>Jenny Zhang</u> (<i>Department of Chemistry, University of Cambridge - UK</i>) Session-K1 Dr. 09:00 - 09:30 <u>David Mitzi</u> (<i>Duke University</i>) Session-K2 Organic-Inorganic Perovskites: Unrivaled Versatility for Semiconductor Design and Fabrication
10:30 - 11:00	Coffee Break
12:30 - 14:00	Lunch
	PERFuDe 1.3 Chair: David Mitzi 15:00 - 15:30 <u>jacky even</u> (<i>Univ Rennes, INSA Rennes, CNRS, Institut FOTON - UMR6082, F-35000 RENNES</i>) 1.3-I1 About the Usefulness of Symmetry and Empirical Approaches for the Theoretical Study of Bulk Halide Perovskites and Halide Perovskite Nanostructures
15:30 - 16:00	Coffee Break
	PERFuDe 1.4 Chair: David Mitzi 16:00 - 16:30 <u>Constantinos Stoumpos</u> (<i>Department of Materials Science and Technology, University of Crete, 71003 Heraklion, Crete, Greece</i>) 1.4-I1 Structure-Property Relations Two-Dimensional Halide Perovskites 16:30 - 16:45 <u>Ferdinand Grozema</u> (<i>Department of Chemical Engineering, Delft University of Technology, The Netherlands</i>) 1.4-O1 Towards Two-dimensional Hybrid Perovskites with Functional Organic Components 16:45 - 17:00 <u>Jovana Milic</u> (<i>Laboratory of Photonics and Interfaces, EPFL, Switzerland</i>), Dominik Kubicki, Lyndon Emsley, 1.4-O2 Michael Graetzel Supramolecular Engineering of Layered Hybrid Perovskite Materials for Stable Perovskite Solar Cells
November 7th - Day 5 (Thursday)	
	PERFuDe 2.1 Chair: Constantinos Stoumpos 09:00 - 09:30 <u>Piers Barnes</u> (<i>Imperial College London</i>) 2.1-I2 The Physics of Perovskite Devices and Interfaces 09:30 - 09:45 <u>Thomas Unold</u> (<i>Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>), Martin Stolterfoht, Christian Wolff, Pietro Caprioglio, Jose Marquez-Prieto, Sergej Levchenko, Dieter Neher, Thomas Kirchartz 2.1-O1 Photoluminescence Quantum Efficiency, Carrier Lifetime and Quasi-Fermi Level Splitting in Highly-efficient Perovskite Solar Cells

09:45 - 10:00 2.1-O2	<u>Paul Fassl</u> (<i>Institute of Microstructure Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany</i>), Vincent Lami, Raphael Schmager, David Becker-Koch, Isabel Allegro, Uli Lemmer, Yana Vaynzof, Bryce S. Richards, Ulrich W. Paetzold Modelling Self-Absorption Induced Red-Shift of the Photoluminescence of Perovskite Thin Films to Estimate the Internal Photoluminescence Quantum Efficiency and Escape Probability
10:00 - 10:30 2.1-I1	<u>Kylie Catchpole</u> (<i>The Australian National University</i>) Understanding Interfaces and Transport Layers in Perovskite Solar Cells
10:30 - 11:00	Coffee Break
PERFuDe 2.2 Chair: Piers Barnes	
11:00 - 11:30 2.2-I1	<u>Evelyne Knapp</u> (<i>Institute of Computational Physics, Zurich University of Applied Sciences (ZHAW), 8401 Winterthur (Switzerland)</i>), Andreas Schiller, Martin T. Neukom, Simon Züfle, Beat Ruhstaller Consistent Device Model of a Perovskite Solar Cell for Multiple Experiments
11:30 - 11:45 2.2-O1	<u>Paramvir Ahlawat</u> (<i>Laboratory of Computational Chemistry and Biochemistry, Dept. of Chemistry, Ecole Polytechnique Fédérale de Lausanne</i>), Michele Parrinello, Ursula Rothlisberger Molecular Dynamics Simulations of Nucleation of Lead Halide Perovskites
11:45 - 12:00 2.2-O2	<u>Mykhailo Sytnyk</u> (<i>Institute -Materials for Electronics and Energy Technology, Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Energy Campus Nürnberg, Fürtherstraße 250, Nürnberg 90429, Germany</i>), AmirAbbas YousefiAmin, Tim Freund, Wolfgang Heiss, Christina Harreiss, Erdmann Spiecker, Valentine V. Volobuev, Jędrzej Korczak, Tomasz Story, Gunther Springholz, Annemarie Pfnür, Klaus Götz, Tobias Unruh, Kamalpreet Singh, Oleksandr Voznyy, Ole Lytken Epitaxial Metal Halide Perovskites by InkJet Printing
12:00 - 12:15 2.2-O3	<u>Florian Mathies</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>), Hampus Näsström, Oleksandra Shargaieva, Gopinath Paramasivam, Eva Unger Opportunities of Inkjet-printed Organic Metal Halide Perovskite Solar Cells
12:15 - 12:30 2.2-O4	<u>Kai Oliver Brinkmann</u> (<i>Institute of Electronic Devices, University of Wuppertal, Germany</i>), Tobias Gahlmann, Junjie He, Christian Tückmantel, Manuel Theisen, Tim Becker, Johannes Bahr, Cedric Kreusel, Jun Song, Junle Qu, Thomas Riedl Intrinsic ALD Barriers Enable Processing on Top of Perovskite Solar Cells from Environmentally Friendly Solvents
12:30 - 14:00	Lunch
PERFuDe 2.3 Chair: Evelyne Knapp	
14:00 - 14:30 2.3-I1	<u>Marco Bernardi</u> (<i>Department of Applied Physics, California Institute of Technology,</i>) Advances in Computing Charge Transport in Perovskite Materials from First Principles
14:30 - 14:45 2.3-O1	<u>Géraud Delport</u> (<i>Optoelectronics Group, Cavendish Laboratory, University of Cambridge, UK.</i>), Camille Stavrakas, Edward Barnard, Miguel Anaya, Samuel D. Stranks Understanding the Influence of the Microscopic Structure of 2D and 3D Perovskites Materials on the Local Diffusion of Carriers.
14:45 - 15:00 2.3-O3	<u>Athanasios Koliogiorgos</u> (<i>Faculty of Electrical Engineering, Czech Technical University in Prague, Prague, Czech Republic</i>), Christos Garoufalos, Iosif Galanakis, Sotirios Baskoutas Electronic and Optical Properties of ABX ₃ (A = Cs, CH ₃ NH ₃ /B = Ge, Pb, Sn, Ca, Sr/X = Cl, Br, I) Perovskite Quantum Dots
15:00 - 15:15 2.3-O4	<u>Joachim Breternitz</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>), Frederike Lehmann, Sarah Barnett, Hariott Nowell, Susan Schorr Crystallography of Hybrid Halide Perovskites: Fundamental Reasoning of Ferroelectricity in MAPbI ₃
15:15 - 15:30 2.3-O2	<u>Bogdan Benin</u> (<i>Institute of Inorganic Chemistry, Department of Chemistry and Applied Bioscience, ETH Zurich, 8093 Zurich, Switzerland</i>), Sergii Yakunin, Dmitry Dirin, Maksym Kovalenko Low-dimensional Tin-halides: Properties and Novel Applications

15:30 - 16:00	Coffee Break
	PERFuDe 2.4 Chair: Kylie Catchpole
16:00 - 16:30 2.4-I1	<u>Iván Mora-Seró</u> (<i>Institute of Advanced Materials (INAM), Universitat Jaume I</i>) Characterization of Transport and Recombination in Perovskite Solar Cells by Impedance Spectroscopy
16:30 - 16:45 2.4-O1	<u>Firouzeh Ebadi</u> (<i>Laboratory of Photomolecular Science (LSPM), Institute of Chemical Sciences and Engineering, School of Basic Sciences, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland.</i>), Nima taghavinia, Raheleh mohammadpour, Anders Hagfeldt, Wolfgang Tress Origin of apparent light-enhanced and negative capacitance in perovskite solar cells
16:45 - 17:00 2.4-O2	<u>Laura Canil</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>), Antonio Abate Perovskite Work Function Tuning through Self-Assembling Monolayers
17:00 - 19:00	Poster Session
November 8th - Day 6 (Friday)	
	Plenary Session Chair: Paulina Plochocka
09:00 - 09:30 Session-K1	<u>Dmitri Talapin</u> (<i>Department of Chemistry, University of Chicago, Chicago, Illinois 60637, USA</i>) Self-organization of Electrostatically and Sterically Stabilized Colloidal Nanocrystals: The Roles of Topology, Image Charges and Non-classical Nucleation
09:00 - 09:30 Session-K2	<u>Xiaoyang Zhu</u> (<i>Department of Chemistry, Columbia University, New York, New York 10027, United States</i>) Ferroelectric Polarons in Lead Halide Perovskites
	PERFuDe 3.1 Chair: Marco Bernardi
09:30 - 10:00 3.1-I1	<u>Daniele Meggiolaro</u> (<i>CompuNet, Istituto Italiano di Tecnologia, Genova, Italy</i>) Defects, Polarons and Surfaces in Metal Halides Perovskites: A DFT Perspective
10:00 - 10:15 3.1-O1	<u>Philippe Tamarat</u> (<i>LP2N, Univ. Bordeaux, IOGS & CNRS, Talence (France)</i>) Band-edge Exciton Fine Structure in Lead-halide Perovskite Nanocrystals
10:15 - 10:30 3.1-O2	Géraud Delport, Gabriel Chehade, Ferdinand Lédée, Hiba Diab, Cosme Milési-Brault, Gaëlle Trippé-Allard, Jacky Even, Jean-Sébastien Lauret, Emmanuelle Deleporte, <u>Damien Garrot</u> (<i>Groupe d'Etude de la Matière Condensée, CNRS, Université de Versailles Saint-Quentin-en-Yvelines, 45 Avenue des Etats Unis, Université Paris-Saclay, 78035, Versailles</i>) Exciton-Exciton Annihilation in Two-dimensional Halide Perovskites
10:30 - 11:00	Coffee Break
	PERFuDe 3.2 Chair: Daniele Meggiolaro
11:00 - 11:30 3.2-I1	<u>Antonio Guerrero</u> (<i>1 Institute of Advanced Materials (INAM), Universitat Jaume I, Castellon, 12006 (Spain)</i>) Role of Migrating Ions in Lead Halide Perovskites at Modifying the External Interfaces
11:30 - 11:45 3.2-O1	Rajendrakumar Gunasekaran, <u>Prabakar Kandsamy</u> (<i>Pusan National University</i>) Open Air Processed Perovskite Solar Cells using Dopant-Free and High Mobility Hydrophobic hole-transporting materials
11:45 - 12:00 3.2-O2	<u>Lara Perrin</u> (<i>Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, France</i>), Manon Spalla, Emilie Planes, Muriel Matheron, Solenn Berson, Lionel Flandin Protective role of gold in case of tert-butylpyridine doped hole transporting layers via gold-pyridine complexes formation: highlighting of a direct impact on perovskite stability

12:00 - 12:15 3.2-O3	<u>Felix Lang</u> (<i>Cavendish Laboratory, Department of Physics, University of Cambridge, UK</i>), Marko Jošt, Kyle Frohna, Amran A. Ashouri, Alan R. Bowman, Tobias Bertram, Anna Belen Morales-Vilches, Elizabeth M. Tennyson, Krzysztof Galkowski, Bernd Stannowski, Christian A. Kaufmann, Rutger Schlatmann, Jürgen Bundesmann, Andrea Denker, Jörg Rappich, Steve Albrecht, Heinz-Christoph Neitzert, Norbert H. Nickel, Samuel D. Stranks Radiation Hardness of Perovskite/Silicon and Perovskite/CIGS Tandem Solar Cells under Proton Irradiation
12:15 - 12:30 3.2-O4	<u>Wouter Van Gompel</u> (<i>UHasselt – Hasselt University, Institute for Materials Research (IMO-IMOMEC), Agoralaan – Building D, 3590 Diepenbeek, Belgium</i>), Roald Herckens, Bart Ruttens, María Gélvez-Rueda, Nadège Marchal, David Beljonne, Kristof Van Hecke, Laurence Lutsen, Dirk Vanderzande Towards a Functional Organic Layer for Low-Dimensional Hybrids
12:30 - 14:00	Lunch
	PERFuDe 3.3 Chair: Iván Mora-Seró
14:00 - 14:30 3.3-I1	<u>Marina Filip</u> (<i>Molecular Foundry, Lawrence Berkeley National Laboratory</i>), Jonah Haber, Jeffrey Neaton Excitonic Properties of Lead-Halide Perovskites from First Principles Computational Modeling
14:30 - 14:45 3.3-O1	<u>Linn Leppert</u> (<i>Institute of Physics, University of Bayreuth, Germany</i>) Optoelectronic Properties of Halide Perovskites with ab Initio Many-body Perturbation Theory
14:45 - 15:00 3.3-O2	<u>Sahel Ashhab</u> (<i>Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha</i>) Intermediate-scale Simulations of Lead-halide Perovskites Using Tight-binding and Spin Models
15:00 - 15:30 3.3-I2	<u>Paulina Plochocka</u> (<i>Laboratoire National des Champs Magnétiques Intenses, CNRS</i>) Excitons and Polarons in Hybrid Perovskite
15:30 - 16:00	Coffee Break
	PERFuDe 3.4 Chair: Marina Filip
16:00 - 16:15 3.4-O3	<u>Arpit Mishra</u> (<i>EDF R&D, Department EFES, EDF Lab – Paris Saclay, France</i>), Philippe Baranek, Andrei Postnikov First-principles Investigation of CO₂, CO and O₂ Adsorption on Perfect and Defective CsPbX₃ (X= Cl, Br, I) Surfaces.
16:15 - 16:30 3.4-O4	<u>RAVI KASHIKAR</u> (<i>Indian Institut of Technology Madras</i>), Mayank Gupta, B. R. K. Nanda Occurence of Invariant Dirac States in CsSnI₃ Polymorphs Under Strain
16:30 - 16:45 3.4-O1	<u>Kunnummal M. Muhammed Salim</u> (<i>Institute of Advanced Materials (INAM), Universitat Jaume I</i>), Sofia Masi, Ehsan Hassanabadi, Azhar Fakharuddin, Ivan Mora Sero Electron Transport Layer and Buffer Layer Optimization for Highly Efficient CsPbI₃ Quantum Dot Based Light Emitting Diodes
16:45 - 17:00 3.4-O2	<u>Qiong Wang</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>) Investigation of Charge Extraction and Accumulation in Perovskite Solar Cells at the Interface of Perovskite and Hole Transport Layer.