

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 5 Chair: Jacky Even Room: Plenum
09:00 - 09:30	<u>David Mitzi</u> (<i>Duke University</i>)
5-K1	Organic-Inorganic Perovskites: Unrivaled Versatility for Semiconductor Design and Fabrication
	Plenary Session 6 Chair: Erwin Reisner Room: Breakout 4
09:00 - 09:30	<u>Jenny Zhang</u> (<i>Department of Chemistry, University of Cambridge - UK</i>)
6-K1	Semi-artificial Photosynthesis: a Platform for Studying and Wiring Photosynthesis
10:30 - 11:00	Coffee Break
12:30 - 14:00	Lunch
	PERFuDe 1.3 Chair: David Mitzi Room: Breakout 4
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 Room: Breakout 4
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, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland</i>), Dominik Kubicki, Lyndon Emsley, Michael Graetzel
1.4-O2	Supramolecular Engineering of Layered Hybrid Perovskite Materials for Stable Perovskite Solar Cells
November 7th - Day 5 (Thursday)	
	PERFuDe 2.1 Chair: Constantinos Stoumpos Room: Plenum
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 2.1-O1	<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 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 Room: Plenum
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>Friedrich Alexander University Erlangen-Nuremberg</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: Jovana Milic Room: Plenum
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 Garoufalidis, 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	<u>Joachim Breternitz</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>), Frederike Lehmann, Sarah Barnett, Hariott Nowell, Susan Schorr
2.3-O4	Crystallography of Hybrid Halide Perovskites: Fundamental Reasoning of Ferroelectricity in MAPbI ₃
15:15 - 15:30	<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
2.3-O2	Low-dimensional Tin-halides: Properties and Novel Applications
15:30 - 16:00	Coffee Break
	PERFuDe 2.4 Chair: Kylie Catchpole Room: Plenum
16:00 - 16:30	<u>Iván Mora-Seró</u> (<i>Universitat Jaume I, Institute of Advanced Materials (INAM) - Spain</i>)
2.4-I1	Characterization of Transport and Recombination in Perovskite Solar Cells by Impedance Spectroscopy
16:30 - 16:45	
16:45 - 17:00	<u>Laura Canil</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>), Antonio Abate
2.4-O1	Work Function Tuning through Self-Assembling Monolayers of Fluorinated Molecules
17:00 - 19:00	Poster Session
November 8th - Day 6 (Friday)	
	Plenary Session 7 Chair: Paulina Plochocka Room: Plenum
09:00 - 09:30	<u>Xiaoyang Zhu</u> (<i>Department of Chemistry, Columbia University, New York, New York 10027, United States</i>)
7-K1	Ferroelectric Polarons in Lead Halide Perovskites
	Plenary Session 8 Chair: Ivan Infante Room: Breakout 4
09:00 - 09:30	<u>Dmitri Talapin</u> (<i>Department of Chemistry, University of Chicago, Chicago, Illinois 60637, USA</i>)
8-K1	Self-organization of Electrostatically and Sterically Stabilized Colloidal Nanocrystals: The Roles of Topology, Image Charges and Non-classical Nucleation
	PERFuDe 3.1 Chair: Marco Bernardi Room: Plenum
09:30 - 10:00	<u>Daniele Meggiolaro</u> (<i>CompuNet, Istituto Italiano di Tecnologia, Genova, Italy</i>)
3.1-I1	Defects, Polarons and Surfaces in Metal Halides Perovskites: A DFT Perspective
10:00 - 10:15	<u>Philippe Tamarat</u> (<i>LP2N, Univ. Bordeaux, IOGS & CNRS, Talence (France)</i>)
3.1-O1	Band-edge Exciton Fine Structure in Lead-halide Perovskite Nanocrystals
10:15 - 10:30	Géraud Delport, Gabriel Chehade, Ferdinand Lédée, Hiba Diab, Cosme Milési-Brault, Gaëlle Trippé-Allard,
3.1-O2	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 Room: Plenum
11:00 - 11:30	<u>Antonio Guerrero</u> (<i>Universitat Jaume I, Institute of Advanced Materials (INAM) - Spain</i>)
3.2-I1	Role of Migrating Ions in Lead Halide Perovskites at Modifying the External Interfaces

11:30 - 11:45	Rajendrakumar Gunasekaran, <u>Prabakar Kandsamy</u> (<i>Pusan National University</i>)
3.2-O1	Open Air Processed Perovskite Solar Cells using Dopant-Free and High Mobility Hydrophobic hole-transporting materials
11:45 - 12:00	<u>Lara Perrin</u> (<i>Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, France</i>), Manon
3.2-O2	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	<u>Felix Lang</u> (<i>Cavendish Laboratory, Department of Physics, University of Cambridge, UK</i>), Marko Jošt, Kyle
3.2-O3	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	<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
3.2-O4	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 Room: Plenum
14:00 - 14:30	<u>Marina Filip</u> (<i>Molecular Foundry, Lawrence Berkeley National Laboratory</i>), Jonah Haber, Jeffrey Neaton
3.3-I1	Excitonic Properties of Lead-Halide Perovskites from First Principles Computational Modeling
14:30 - 14:45	<u>Linn Leppert</u> (<i>Institute of Physics, University of Bayreuth, Germany</i>)
3.3-O1	Optoelectronic Properties of Halide Perovskites with ab Initio Many-body Perturbation Theory
14:45 - 15:00	<u>Sahel Ashhab</u> (<i>Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha</i>)
3.3-O2	Intermediate-scale Simulations of Lead-halide Perovskites Using Tight-binding and Spin Models
15:00 - 15:30	<u>Paulina Plochocka</u> (<i>Laboratoire National des Champs Magnétiques Intenses, CNRS</i>)
3.3-I2	Excitons and Polarons in Hybrid Perovskite
15:30 - 16:00	Coffee Break
	PERFuDe 3.4 Chair: Marina Filip Room: Plenum
16:00 - 16:15	<u>Arpit Mishra</u> (<i>EDF R&D, Department EFES, EDF Lab – Paris Saclay, France</i>), Philippe Baranek, Andrei
3.4-O3	Postnikov First-principles Investigation of CO ₂ , CO and O ₂ Adsorption on Perfect and Defective CsPbX ₃ (X= Cl, Br, I) Surfaces.
16:15 - 16:30	<u>RAVI KASHIKAR</u> (<i>Indian Institut of Technology Madras</i>), Mayank Gupta, B. R. K. Nanda
3.4-O4	Occurrence of Invariant Dirac States in CsSnI ₃ polymorphs Under Strain
16:30 - 16:45	<u>Kunnummal M. Muhammed Salim</u> (<i>Universitat Jaume I, Institute of Advanced Materials (INAM) - Spain</i>), Sofia
3.4-O1	Masi, Ehsan Hassanabadi, Azhar Fakharuddin, Ivan Mora Sero Electron Transport Layer and Buffer Layer Optimization for Highly Efficient CsPbI ₃ Quantum Dot Based Light Emitting Diodes
16:45 - 17:00	<u>Qiong Wang</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i>)
3.4-O2	Investigation of Charge Extraction and Accumulation in Perovskite Solar Cells at the Interface of Perovskite and Hole Transport Layer.

Poster Contribution

327	<u>Konstantin Schötz</u> (<i>Soft Matter Optoelectronics, University of Bayreuth, Germany</i>), Abdelrahman Askar, Wei Peng, Dominik Seeberger, Tanaji P. Guijar, Mukundan Thelakkat, Anna Köhler, Sven Hüttner, Osman M. Bakr, Karthik Shankar, Fabian Panzer Understanding double peak emission in lead halide perovskites
330	Taisuke Matsui, Ieva Petrikyte, Tadas Malinauskas, Konrad Domanski, Maryte Daskeviciene, <u>Matas Steponaitis</u> (<i>Department of Organic Chemistry, Kaunas University of Technology, Radvilenu pl. 19, Kaunas, 50254, Lithuania</i>), Paul Gratia, Wolfgang Tress, Juan-Pablo Correa-Baena, Antonio Abate, Anders Hagfeldt, Michael Graetzel, Mohammad Khaja Nazeeruddin, Vytautas Getautis, Michael Saliba Polymeric triphenylamine derivatives for perovskite solar cells
338	<u>Muhammad Sultan</u> (<i>Nanoscience and Technology Department, National Center for Physics, Quaid-I-Azam University Islamabad, Pakistan</i>), Irfan Haider, Azhar Fakhruddin, Lukas Schmidt-Mende Effect of interfacial oxygen stoichiometry on performance of perovskite solar cells
358	<u>Laurence LUTSEN</u> (<i>IMEC, Imomec, Diepenbeek (Belgium)</i>), Dirk VANDERZANDE, Wouter Van Gompel, Roald Herckens, Paul-Henri Denis, Martijn Mertens, Tom Aernouts, Jan D'Haen, Bart Ruttens, Kristof Van Hecke Towards 2D Layered Hybrid Perovskites With Enhanced Functionality.
377	<u>Ernestas Kasparavičius</u> (<i>Faculty of Chemical Technology, Kaunas University of Technology, Radvilėnų pl. 19, Kaunas</i>), Tadas Malinauskas, Vytautas Getautis Stability of Oxidized Spiro-MeOTAD Under Influence of Perovskite and its Components
387	<u>Ioannis Papadas</u> (<i>Cyprus University of Technology</i>), Apostolos Ioakeimidis, Gerasimos Armatas, Stelios Choulis Combustion Synthesized NiCo ₂ O ₄ Hole Transport Layer for Inverted Perovskite Solar Cells
414	<u>Mariia Kramarenko</u> (<i>ICFO-Institut de Ciències Fòtiques, The Barcelona Institute of Science and Technology</i>), Catarina G. Ferreira, Guillermo Martínez-Denegri, Constanza Sansierra, Johann Toudert, Jordi Martorell Interplay of Fluorescence Quantum Yield and Photovoltaic Parameters of Perovskite Solar Cells
417	<u>Hailong Yuan</u> (<i>Institut des Matériaux Jean Rouxel, UMR-CNRS 6502, Université de Nantes, 2 rue de la Houssinière, BP 32229, 44322 Nantes Cedex 3, France</i>), Florian Massuyeau, Romain Gautier, Michael Paris Manganese-doped Lead Halide White Phosphors with High Efficiency and Ultra High Color Rendering
434	<u>Barbara Primera Darwich</u> (<i>Laboratory for Molecular Engineering of Optoelectronic Nanomaterials (LIMNO), École Polytechnique Fédérale de Lausanne (EPFL), , Switzerland</i>), Han-Hee Cho, Nestor Guijarro, Liang Yao, Kevin Sivula, Jun-Ho Yum Expanding the functionality of thiophenes in the quest for halide perovskite stabilization
440	<u>Hamid Ghaithan</u> (<i>Physics and Astronomy, Science Collage, King Saud University</i>), Zeyad Alahmed, Saif Qaid, Mahmoud Hezam, Abdullah Aldwayyan Density Functional Theory Investigation of Structural, Electronic, and Optical Properties of CsPb(I _{1-x} Br _x) ₃ Perovskite