

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 Session-K1	<u>Jenny Zhang</u> (<i>Department of Chemistry, University of Cambridge - UK</i>) Dr.
09:00 - 09:30 Session-K2	<u>David Mitzi</u> (<i>Duke University</i>) Organic-Inorganic Perovskites: Unrivalled Versatility for Semiconductor Design and Fabrication
10:30 - 11:00	Coffee Break
12:30 - 14:00	Lunch
	PERFuDe 1.3
15:00 - 15:30 1.3-I1	<u>jacky even</u> (<i>Univ Rennes, INSA Rennes, CNRS, Institut FOTON - UMR6082, F-35000 RENNES</i>) 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
16:00 - 16:30 1.4-I1	<u>Constantinos Stoumpos</u> (<i>Department of Materials Science and Technology, University of Crete, 71003 Heraklion, Crete, Greece</i>) Structure-Property Relations Two-Dimensional Halide Perovskites
16:30 - 16:45 1.4-O1	<u>Ferdinand Grozema</u> (<i>Department of Chemical Engineering, Delft University of Technology, The Netherlands</i>) Towards Two-dimensional Hybrid Perovskites with Functional Organic Components
16:45 - 17:00 1.4-O2	<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 Supramolecular Engineering of Layered Hybrid Perovskite Materials for Stable Perovskite Solar Cells
November 7th - Day 5 (Thursday)	
	PERFuDe 2.1
09:00 - 09:30 2.1-I2	<u>Piers Barnes</u> (<i>Imperial College London</i>) 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 2.1-02	<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 2.1-11	<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	
11:00 - 11:30 2.2-11	<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 2.2-01	<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 2.2-02	<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 2.2-03	<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 2.2-04	<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	
14:00 - 14:30 2.3-11	<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 2.3-01	<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 2.3-03	<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 2.3-04	<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 2.3-02	<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

- 16:00 - 16:30 Iván Mora-Seró (*Institute of Advanced Materials (INAM), Universitat Jaume I*)
2.4-I1 Characterization of Transport and Recombination in Perovskite Solar Cells by Impedance Spectroscopy
- 16:30 - 16:45 Firouzeh Ebadi (*Laboratory of Photomolecular Science (LSPM), Institute of Chemical Sciences and Engineering, School of Basic Sciences, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland.*), Nima taghavinia, Raheleh mohammadpour, Anders Hagfeldt, Wolfgang Tress
2.4-O1 Origin of apparent light-enhanced and negative capacitance in perovskite solar cells
- 16:45 - 17:00 Laura Canil (*Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany*), Antonio Abate
2.4-O2 Work Function Tuning through Self-Assembling Monolayers of Fluorinated Molecules

17:00 - 19:00 **Poster Session**

November 8th - Day 6 (Friday)

Plenary Session

- 09:00 - 09:30 Dmitri Talapin (*Department of Chemistry, University of Chicago, Chicago, Illinois 60637, USA*)
Session-K1 Self-organization of Electrostatically and Sterically Stabilized Colloidal Nanocrystals: The Roles of Topology, Image Charges and Non-classical Nucleation
- 09:00 - 09:30 Xiaoyang Zhu (*Department of Chemistry, Columbia University, New York, New York 10027, United States*)
Session-K2 Ferroelectric Polarons in Lead Halide Perovskites

PERFuDe 3.1

- 09:30 - 10:00 Daniele Meggiolaro (*CompuNet, Istituto Italiano di Tecnologia, Genova, Italy*)
3.1-I1 Defects, Polarons and Surfaces in Metal Halides Perovskites: A DFT Perspective
- 10:00 - 10:15 Philippe Tamarat (*LP2N, Univ. Bordeaux, IOGS & CNRS, Talence (France)*)
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, Damien Garrot (*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*)
Exciton-Exciton Annihilation in Two-dimensional Halide Perovskites

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

PERFuDe 3.2

- 11:00 - 11:30 Antonio Guerrero (*1 Institute of Advanced Materials (INAM), Universitat Jaume I, Castellon, 12006 (Spain)*)
3.2-I1 Role of Migrating Ions in Lead Halide Perovskites at Modifying the External Interfaces
- 11:30 - 11:45 Rajendrakumar Gunasekaran, Prabakar Kandsamy (*Pusan National University*)
3.2-O1 Open Air Processed Perovskite Solar Cells using Dopant-Free and High Mobility Hydrophobic hole-transporting materials
- 11:45 - 12:00 Lara Perrin (*Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, France*), 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 Felix Lang (*Cavendish Laboratory, Department of Physics, University of Cambridge, UK*), 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 **Wouter Van Gompel** (*UHasselt – Hasselt University, Institute for Materials Research (IMO-IMOMEC), Agoralaan – Building D, 3590 Diepenbeek, Belgium*), 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

14:00 - 14:30 **Marina Filip** (*Molecular Foundry, Lawrence Berkeley National Laboratory*), Jonah Haber, Jeffrey Neaton
3.3-I1 Excitonic Properties of Lead-Halide Perovskites from First Principles Computational Modeling

14:30 - 14:45 **Linn Leppert** (*Institute of Physics, University of Bayreuth, Germany*)
3.3-O1 Optoelectronic Properties of Halide Perovskites with ab Initio Many-body Perturbation Theory

14:45 - 15:00 **Sahel Ashhab** (*Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha*)
3.3-O2 Intermediate-scale Simulations of Lead-halide Perovskites Using Tight-binding and Spin Models

15:00 - 15:30 **Paulina Plochocka** (*Laboratoire National des Champs Magnétiques Intenses, CNRS*)
3.3-I2 Excitons and Polarons in Hybrid Perovskite

15:30 - 16:00 **Coffee Break**

PERFuDe 3.4

16:00 - 16:15 **Arpit Mishra** (*EDF R&D, Department EFSE, EDF Lab – Paris Saclay, France*), Philippe Baranek, Andrei Postnikov
3.4-O3 First-principles Investigation of CO₂, CO and O₂ Adsorption on Perfect and Defective CsPbX₃ (X= Cl, Br, I) Surfaces.

16:15 - 16:30 **RAVI KASHIKAR** (*Indian Institut of Technology Madras*), Mayank Gupta, B. R. K. Nanda
3.4-O4 Occurrence of Invariant Dirac States in CsSnI₃ Polymorphs Under Strain

16:30 - 16:45 **Kunnummal M. Muhammed Salim** (*Institute of Advanced Materials (INAM), Universitat Jaume I*), Sofia Masi, Ehsan Hassanabadi, Azhar Fakharuddin, Ivan Mora Sero
3.4-O1 Electron Transport Layer and Buffer Layer Optimization for Highly Efficient CsPbI₃ Quantum Dot Based Light Emitting Diodes

16:45 - 17:00 **Qiong Wang** (*Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany*)
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 **Konstantin Schötz** (*Soft Matter Optoelectronics, University of Bayreuth, Germany*), 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, **Matas Steponaitis** (*Department of Organic Chemistry, Kaunas University of Technology, Radvilenu pl. 19, Kaunas, 50254, Lithuania*), 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