

## 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) |   |
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| 08:45 - 09:00                    | <b>Announcement of the day &amp; Presentation of NFM20 /Plenum-Room B4</b>  |
|                                  | <b>Plenary Session 5 / Plenum</b><br>Chair: Jacky Even<br>Room: Plenum  |
| 09:00 - 09:30                    | <u>David Mitzi</u> ( <i>Duke University</i> )   |
| Plenum-K1                        | Organic-Inorganic Perovskites: Unrivaled Versatility for Semiconductor Design and Fabrication   |
|                                  | <b>Plenary Session 6 / Room B4</b><br>Chair: Erwin Reisner<br>Room: Breakout 4  |
| 09:00 - 09:30                    | <u>Jenny Zhang</u> ( <i>Department of Chemistry, University of Cambridge - UK</i> )   |
| B4-K1                            | Semi-artificial Photosynthesis: a Platform for Studying and Wiring Photosynthesis   |
| 10:30 - 11:00                    | <b>Coffee Break</b>   |
| 12:30 - 14:00                    | <b>Lunch</b>  |
|                                  | <b>PERFuDe 1.3 / Room B4</b><br>Chair: David Mitzi<br>Room: Breakout 4  |
| 15:00 - 15:30                    | <u>jacky even</u> ( <i>Univ Rennes, INSA Rennes, CNRS, Institut FOTON - UMR6082, F-35000 RENNES</i> )   |
| B4-11                            | About the Usefulness of Symmetry and Empirical Approaches for the Theoretical Study of Bulk Halide Perovskites and Halide Perovskite Nanostructures   |
| 15:30 - 16:00                    | <b>Coffee Break</b>   |
|                                  | <b>PERFuDe 1.4 / Room B4</b><br>Chair: David Mitzi<br>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> )   |
| B4-11                            | Structure-Property Relations Two-Dimensional Halide Perovskites   |
| 16:30 - 16:45                    | <u>Ferdinand Grozema</u> ( <i>Delft University of Technology (TU Delft), The Netherlands</i> )  |
| B4-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 |
| B4-O2                            | Supramolecular Engineering of Layered Hybrid Perovskite Materials for Stable Perovskite Solar Cells   |
| November 7th - Day 5 (Thursday)  |   |
|                                  | <b>PERFuDe 2.1 / Plenum</b><br>Chair: Constantinos Stoumpos<br>Room: Plenum   |

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| 09:00 - 09:30  | <u>Piers Barnes</u> ( <i>Imperial College London</i> )  |
| Plenum-I2  | The Physics of Perovskite Devices and Interfaces  |
| 09:30 - 09:45  | <u>Thomas Unold</u> ( <i>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  |
| Plenum-O1  | Photoluminescence Quantum Efficiency, Carrier Lifetime and Quasi-Fermi Level Splitting in Highly-efficient Perovskite Solar Cells   |
| 09:45 - 10:00  | <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 Schmagar, David Becker-Koch, Yana Vaynzof, Bryce S. Richards, Ulrich W. Paetzold, Ian Howard, Felix Berger, Lukas Falk, Jana Zaumseil       |
| Plenum-O2  | 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  | <u>Kylie Catchpole</u> ( <i>The Australian National University</i> )  |
| Plenum-I1  | Understanding Interfaces and Transport Layers in Perovskite Solar Cells   |
| 10:30 - 11:00  | <b>Coffee Break</b>   |
| <b>PERFuDe 2.2 / Plenum</b><br>Chair: Piers Barnes<br>Room: Plenum |   |
| 11:00 - 11:30  | <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   |
| Plenum-I1  | Consistent Device Model of a Perovskite Solar Cell for Multiple Experiments   |
| 11:30 - 11:45  | <u>Paramvir Ahlawat</u> ( <i>Laboratory of Computational Chemistry and Biochemistry, Dept. of Chemistry, Ecole Polytechnique Fédérale de Lausanne</i> ), Michele Parrinello, Ursula Rothlisberger   |
| Plenum-O1  | Molecular Dynamics Simulations of Nucleation of Lead Halide Perovskites   |
| 11:45 - 12:00  | <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 |
| Plenum-O2  | Epitaxial Metal Halide Perovskites by InkJet Printing   |
| 12:00 - 12:15  | <u>Florian Mathies</u> ( <i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i> ), Hampus Näsström, Oleksandra Shargaieva, Gopinath Paramasivam, Eva Unger   |
| Plenum-O3  | Opportunities of Inkjet-printed Organic Metal Halide Perovskite Solar Cells   |
| 12:15 - 12:30  | <u>Kai Oliver Brinkmann</u> ( <i>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  |
| Plenum-O4  | Intrinsic ALD Barriers Enable Processing on Top of Perovskite Solar Cells from Environmentally Friendly Solvents  |
| 12:30 - 14:00  | <b>Lunch</b>  |
| <b>PERFuDe 2.3 / Plenum</b><br>Chair: Jovana Milic<br>Room: Plenum |   |
| 14:00 - 14:30  | <u>Marco Bernardi</u> ( <i>Department of Applied Physics, California Institute of Technology,</i> )   |
| Plenum-I1  | Advances in Computing Charge Transport in Perovskite Materials from First Principles  |
| 14:30 - 14:45  | <u>Géraud Delport</u> ( <i>Optoelectronics Group, Cavendish Laboratory, University of Cambridge, UK.</i> ), Camille Stavrakas, Edward Barnard, Miguel Anaya, Samuel D. Stranks  |
| Plenum-O1  | Understanding the Influence of the Microscopic Structure of 2D and 3D Perovskites Materials on the Local Diffusion of Carriers.   |
| 14:45 - 15:00  | <u>Athanasios Koliogiorgos</u> ( <i>Faculty of Electrical Engineering, Czech Technical University in Prague, Prague, Czech Republic</i> ), Christos Garoufalis, Iosif Galanakis, Sotirios Baskoutas   |
| Plenum-O3  | Electronic and Optical Properties of ABX <sub>3</sub> (A = Cs, CH <sub>3</sub> NH <sub>3</sub> /B = Ge, Pb, Sn, Ca, Sr/X = Cl, Br, I) Perovskite Quantum Dots   |

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| 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   |
| Plenum-O4   | Crystallography of Hybrid Halide Perovskites: Fundamental Reasoning of Ferroelectricity in MAPbI <sub>3</sub>   |
| 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   |
| Plenum-O2   | Low-dimensional Tin-halides: Properties and Novel Applications  |
| 15:30 - 16:00   | <b>Coffee Break</b>   |
| <b>PERFuDe 2.4 / Plenum</b><br>Chair: Kylie Catchpole<br>Room: Plenum         |   |
| 16:00 - 16:30   | <u>Paulina Plochocka</u> ( <i>Laboratoire National des Champs Magnétiques Intenses, CNRS</i> )  |
| Plenum-I1   | Excitons and Polarons in Hybrid Perovskite  |
| 16:30 - 16:45   | <u>Laura Canil</u> ( <i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i> ), Antonio Abate   |
| Plenum-O1   | Work Function Tuning through Self-Assembling Monolayers of Fluorinated Molecules  |
| 16:45 - 17:00   |   |
| 17:00 - 19:00   | <b>Poster Session</b>   |
| <b>November 8th - Day 6 (Friday)</b>  |   |
| 08:45 - 09:00   | <b>Announcement of the day / Plenum-Room B4</b>   |
| <b>Plenary Session 7 / Plenum</b><br>Chair: Wolfgang Tress<br>Room: Plenum    |   |
| 09:00 - 09:30   | <u>Xiaoyang Zhu</u> ( <i>Department of Chemistry, Columbia University, New York, New York 10027, United States</i> )  |
| Plenum-K1   | Ferroelectric Polarons in Lead Halide Perovskites   |
| <b>Plenary Session 8 / Room B4</b><br>Chair: Ivan Infante<br>Room: Breakout 4 |   |
| 09:00 - 09:30   | <u>Dmitri Talapin</u> ( <i>Department of Chemistry, University of Chicago, Chicago, Illinois 60637, USA</i> )   |
| B4-K1   | Self-organization of Electrostatically and Sterically Stabilized Colloidal Nanocrystals: The Roles of Topology, Image Charges and Non-classical Nucleation  |
| <b>PERFuDe 3.1 / Plenum</b><br>Chair: Simone Meloni<br>Room: Plenum           |   |
| 09:30 - 10:00   | <u>Antonio Guerrero</u> ( <i>Universitat Jaume I, Institute of Advanced Materials (INAM) - Spain</i> )  |
| Plenum-I1   | Role of Migrating Ions in Lead Halide Perovskites at Modifying the External Interfaces  |
| 10:00 - 10:15   | <u>Philippe Tamarat</u> ( <i>LP2N, Univ. Bordeaux, IOGS &amp; CNRS, Talence (France)</i> )  |
| Plenum-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, 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> ) |
| Plenum-O2   | Exciton-Exciton Annihilation in Two-dimensional Halide Perovskites  |
| 10:30 - 11:00   | <b>Coffee Break</b>   |
| <b>PERFuDe 3.2 / Plenum</b><br>Chair: Didier Mayou<br>Room: Plenum            |   |
| 11:00 - 11:30   | <u>Iván Mora-Seró</u> ( <i>Universitat Jaume I, Institute of Advanced Materials (INAM) - Spain</i> )  |
| Plenum-I1   | Characterization of Transport and Recombination in Perovskite Solar Cells by Impedance Spectroscopy   |

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| 11:30 - 11:45<br>Plenum-O1   | <u>Rajendrakumar Gunasekaran, Prabakar Kandsamy</u> ( <i>Pusan National University</i> )<br>Open Air Processed Perovskite Solar Cells using Dopant-Free and High Mobility Hydrophobic hole-transporting materials  |
| 11:45 - 12:00<br>Plenum-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<br>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<br>Plenum-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<br>Radiation Hardness of Perovskite/Silicon and Perovskite/CIGS Tandem Solar Cells under Proton Irradiation |
| 12:15 - 12:30<br>Plenum-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<br>Towards a Functional Organic Layer for Low-Dimensional Hybrids   |
| 12:30 - 14:00  | <b>Lunch</b>   |
| <b>PERFuDe 3.3 / Plenum</b><br>Chair: Iván Mora-Seró<br>Room: Plenum |  |
| 14:00 - 14:30<br>Plenum-I1   | <u>Marina Filip</u> ( <i>Molecular Foundry, Lawrence Berkeley National Laboratory</i> ), Jonah Haber, Jeffrey Neaton<br>Excitonic Properties of Lead-Halide Perovskites from First Principles Computational Modeling   |
| 14:30 - 14:45<br>Plenum-O1   | <u>Linn Leppert</u> ( <i>Institute of Physics, University of Bayreuth, Germany</i> )<br>Optoelectronic Properties of Halide Perovskites with ab Initio Many-body Perturbation Theory   |
| 14:45 - 15:00<br>Plenum-O2   | <u>Sahel Ashhab</u> ( <i>Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha</i> )<br>Intermediate-scale Simulations of Lead-halide Perovskites Using Tight-binding and Spin Models  |
| 15:00 - 15:30  |  |
| 15:30 - 16:00  | <b>Coffee Break</b>  |
| <b>PERFuDe 3.4 / Plenum</b><br>Chair: Marina Filip<br>Room: Plenum   |  |
| 16:00 - 16:15<br>Plenum-O3   | <u>Arpit Mishra</u> ( <i>EDF R&amp;D, Department EFESE, EDF Lab – Paris Saclay, France</i> ), Philippe Baranek, Andrei Postnikov<br>First-principles Investigation of CO <sub>2</sub> , CO and O <sub>2</sub> Adsorption on Perfect and Defective CsPbX <sub>3</sub> (X= Cl, Br, I) Surfaces.  |
| 16:15 - 16:30<br>Plenum-O4   | <u>RAVI KASHIKAR</u> ( <i>Indian Institut of Technology Madras</i> ), Mayank Gupta, B. R. K. Nanda<br>Occurrence of Invariant Dirac States in CsSnI <sub>3</sub> polymorphs Under Strain   |
| 16:30 - 16:45<br>Plenum-O1   | <u>Kunnummal M. Muhammed Salim</u> ( <i>Universitat Jaume I, Institute of Advanced Materials (INAM) - Spain</i> ), Sofia Masi, Ehsan Hassanabadi, Azhar Fakharuddin, Ivan Mora Sero<br>Electron Transport Layer and Buffer Layer Optimization for Highly Efficient CsPbI <sub>3</sub> Quantum Dot Based Light Emitting Diodes  |
| 16:45 - 17:00<br>Plenum-O2   | <u>Qiong Wang</u> ( <i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany</i> )<br>Investigation of Charge Extraction and Accumulation in Perovskite Solar Cells at the Interface of Perovskite and Hole Transport Layer.  |