**Hybrid Inorganic/Organic Systems**
**for Opto-Electronics**
Collaborative Research Centre 951

HIOS

# Special Colloquium Announcement

### of the Collaborative Research Centre 951
### "Hybrid Inorganic/Organic Systems for Opto-Electronics"

## Philip Schulz

CNRS, Institut Photovoltaique d'Ile de France (IPVF), France

# Halide Perovskites:
# Is it all about the Interfaces?

Time: Tuesday, April 30, 2019, **11:00 s.t.**
Place: IRIS Adlershof, Zum Großen Windkanal 6,
Room 007 (ground floor).

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# Halide Perovskites: Is it all about the Interfaces?

**Philip Schulz**

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My talk will focus on the means and developments to analyze and tailor interfaces in halide perovskite (HaP) based semiconductor devices to gain control over the electronic properties at the nanoscale, as interfacial design routes determine the electronic coupling between the perovskite absorber and adjacent charge extraction and transport layers. On the one hand, the device characteristics can be affected by the alignment of the frontier molecular orbitals of an organic charge transport layers (CTL) with the electronic transport level in the perovskite. On the other hand, the doping type of the substrate underneath can template the doping type of subsequently deposited HaP films. In our studies we elucidated these mechanisms by examining a selection of charge transport layers adjacent to the perovskite film.[1] We reported on the energy level alignment between HaP films and organic charge transport layers, oxide substrates, carbon nanotube thin-films and high-work function $MoO_3$ overlayers. In this talk I will summarize these findings and describe the challenges to generalize these trends as the complex chemistry between HaP layer and adjacent semiconductor often lies at the root of the observed interfacial alignment processes and band bending.[2]

In my talk, I will highlight the use of ultraviolet and X-ray photoemission spectroscopy (UPS/XPS) as well as inverse photoemission spectroscopy (IPES) to determine the surface energetics and electronic energy level alignment at the HaP/CTL interface while at the same time tracking the interface chemistry. This approach, complemented by additional optical spectroscopy and mass spectrometry techniques, enables us to evaluate band offsets in the layer system in face of chemical interactions and changes in the electrostatic potential at the interfaces. The results not only suggest guidelines on how to integrate CTLs into perovskite photovoltaic devices but also explain more generally to what extent the electronic structure of the perovskite is subject to extrinsic perturbations and would ultimately pertain to stability concerns in devices.[3] In our more recent work, we explicitly investigate beam damage in the perovskite layers that exhibit distinct signs of degradation under vacuum conditions and concomitant irradiation with high-energy photons. While we generally intend to avoid these transient effects in our measurements, we can extract additional physical and chemical parameters from the evolution of energy level positions and stoichiometry during the PES measurements, which carries direct implications on the material stability.[4-6]

I will conclude my talk by further exemplify how surface treatment and interfacial design routes can be employed to achieve record power conversion efficiencies in HaP-based quantum dot solar cells.[7] Therein, our approach is driven by a targeted ligand exchange chemistry.[8]

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[2] P. Schulz, D. Cahen, A. Kahn Chem. Rev. **2019**, *119*, 3349-3417

[3] J.A. Christians, P. Schulz, J.S. Tinkham, T.H. Schloemer, S.P. Harvey, B.J. Tremolet de Villiers, A. Sellinger, J J. Berry, J.M. Luther, *Nature Energy* **2018,** *3*, 68-74

[4] K. X. Steirer, P. Schulz, G. Teeter, V. Stevanovic, M. Yang, K. Zhu, J. J. Berry, *ACS Energy Lett.* **2016**, *1*, 360-366

[5] R. A. Kerner, T. Schloemer, P. Schulz, J. J. Berry, J. Schwartz, A. Sellinger, B. P. Rand *J. Mater. Chem. C* **2018**, C8TC04871A

[6] R. A. Kerner, P. Schulz, J. A. Christians, S. B. Dunfield, B. Dou, G. Teeter, J. J. Berry, B. P. Rand, *APL Materials* **2019**, *7*, 041103

[7] E. M. Sanehira, A. R. Marshall, J. A. Christians, S. P. Harvey, P. N. Ciesielski, L. M. Wheeler, P. Schulz, L. Y. Lin, M. C. Beard, J. M. Luther, *Science Adv.* **2017**, *3*, eaao4204

[8] L.M. Wheeler, E.M. Sanehira, A.R. Marshall, P. Schulz, M. Suri, N.C. Anderson, J.A. Christians, D. Nordlund, D. Sokaras, T. Kroll, S.P. Harvey, J.J. Berry, L.Y. Lin, J.M. Luther *J. Am. Chem. Soc*. **2018**, *140*, 10504