Defect Physics and (In)Stability in Metal-halide Perovskite Semiconductors

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Semiconducting metal-halide perovskites present various types of chemical interactions which give them a characteristic fluctuating structure sensitive to the operating conditions of the device, to which they adjust. This makes the control of structure-properties relationship, especially at interfaces where the device realizes its function, the crucial step in order to control devices operation. In particular, given their simple processability at relatively low temperature, one can expect an intrinsic level of structural/chemical disorder of the semiconductor which results in the formation of defects.

Here, first I will present our results on the role of structural and point defects in determining the nature and dynamic of photo-carriers in metal-halide perovskites. Then, I will discuss our understanding of key parameters which must be taken into consideration in order to evaluate the susceptibility of the perovkite crystals (2D and 3D) to the formation of defects, allowing one to proceed through a predictive synthetic procedure. Finally, I will show the correlation between the presence/formation of defects and the observed semiconductor instabilities. Instabilities are manifested as light-induced ion migration and segregation, eventually leading to material degradation under prolonged exposure to light. Understanding, controlling and eventually blocking such material instabilities are fundamental steps towards large scale exploitation of perovskite in optoelectronic devices. By combining photoluminescence measurements under controlled conditions with ab initio simulations we identify photo-instabilities related to competing light-induced formation and annihilation of trap states, disclosing their characteristic length and time scales and the factors responsible for both processes. We show that short range/short time defect annihilation can prevail over defect formation, happening on longer scales, when effectively blocking undercoordinated surface sites, which act as a defect reservoir. By an effective surface passivation strategy we are thus able to stabilize the perovskite layer towards such photo-induced instabilities, leading to improved optoelectronic material quality and enhanced photo-stability in a working solar cell. The proposed strategy represents a simple solution towards longer stability perovskite thin films that could be easily implemented in large scale manufacturing.
Dr. Annamaria Petrozza is Senior Scientist at the Istituto Italiano di Tecnologia. She was awarded a Master of Science in Electronic Engineering at Ecole Supérieure d’Électricité (Paris, France) in 2003 and at Politecnico di Milano in 2014 under the T.I.M.E. (Top Industrial Manager in Europe) program. In 2008 she received her PhD in Physics from the University of Cambridge (UK) with a thesis on the study of optoelectronic processes at organic and hybrid semiconductors interfaces, under the supervision of Dr J.S Kim and Prof Sir R.H. Friend. From 2008 to 2009 she worked as staff scientist at the Sharp Laboratories of Europe, Ltd on the development of new market competitive solar cell technologies. In 2010 she joined the newly founded Center for Nano Science and Technology (CNST) of IIT in Milan. Since 2013 she leads the Advanced Materials for Optoelectronics Research Line at CNST. Her research mainly aims to shed light on optoelectronic mechanisms which are fundamental for the optimization of operational processes of devices made of functional materials, with the goal of improving device efficiency and stability. Annamaria was awarded the “Innovators Under 35 Italy” - MIT Technology Review in 2014 for her pioneer work in the field of perovskite semiconductors. In 2017 she was awarded with an ERC consolidator grant.