INTERFACE EFFECTS ON PEROVSKITE SOLAR CELLS

Ali Akbari[†], Javad Hashemi[†], Edoardo Mosconi[‡], Filippo De Angelis[‡], and Mikko Hakala[†]

[†]Department of Physics, P.O. Box 64, FIN-00014 University of Helsinki, Finland
[‡]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), Istituto CNR di Scienze e Tecnologie Molecolari (ISTM-CNR), Via Elce di Sotto 8, 06123, Perugia, Italy.
email: ali.akbari@helsinki.fi

The recent emergence of perovskite solar cells has revolutionized the field of photovoltaics. Starting from 3.8% efficiency[1], these perovskite solar cells have now reached 20.1% efficiency[2], surpassing other available options for inexpensive solar cell technologies. Interfaces play a pivotal role in the charge transfer occurring in these cells and have been shown to have significant effect also on the cell stability. Hence, one way to further increase the efficiency is to gain control over the effects of interfaces on the cell properties. Although experimentally a careful control of these effects have been pursued[3], present efforts are mostly trial and error in nature and a systematic study on the underlying mechanisms of these effects is still missing.

In this presentation we report the results of our computational studies (density-functional-theory simulations) of the perovskite ($CH_3NH_3PbI_3$) interface with Al_2O_3, and TiO_2, the most commonly used materials in perovskite cells. We will show that the perovskite binds much stronger onto alumina in comparison with the titania. We will examine the nature of the binding and the formed bonds to rationalize this difference. Finally we study the electronic structures of these interfaces and obtain the band bending occurring across the interface. Using this information, we confirm the recent experimental finding[4] that the perovskite (110) plane has a poor conduction band alignment with respect to TiO_2 while the (001) plane has an excellent band alignment.

[1] A. Kojima, K. Teshima, Y. Shirai, and T. Miyasaka, Journal of the American Chemical Society **131**, 6050 (2009).

[2] W. S. Yang, J. H. Noh, N. J. Jeon, Y. C. Kim, S. Ryu, J. Seo, and S. I. Seok, Science **348**, 6240 (2015).

[3] H. Zhou, Q. Chen, G. Li, S. Luo, T. Song, H. Duan, Z. Hong, J. You, Y. Liu, and Y. Yang, Science **345**, 542 (2014).

[4] J. P. Correa Baena, L. Steier, W. Tress, M. Saliba, S. Neutzner, T. Matsui, F. Giordano, T. J. Jacobsson, A. R. Srimath Kandada, S. M. Zakeeruddin, A. Petrozza, A. Abate, M. K. Nazeeruddin, M. Grätzel, A. Hagfeldt, Energy Environ. Sci. **8** 2928 (2015).