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Design of electronic properties in organic materials: combining empirical and computational approaches

Dmitrii F. Perepichka
Department of Chemistry
McGill University

Modern computational methods have become reliable and accurate predictors of molecular properties and, as such, powerful design tools in the hands of organic chemists. We are particularly interested in the design of materials with unusual electronic properties. However, the behavior of these materials in electronic devices depends not only on the individual properties of molecules, but also on "harder to predict" supramolecular interactions as well as interactions with the "outside" world, *eg*. metal contacts. Thus, empirical search is still a necessary element of discovery.

In this lecture, I will show the use and limitations of density-functional theory (DFT) calculations in the design of new organic electronic materials, including Aviram-Ratner unimolecular diodes, molecular semiconductors [1], low band-gap polymers [2], and surface-confined organic nanostructures [3,4]. I will specifically highlight how calculations can help rationalize the "unusual behavior" observed in the studied materials.

In the last part of the lecture, I will briefly describe our work on solution processable up-converting inorganic materials. Building upon the pioneering work by Capobianco *et al.*, we have recently demonstrated the synthesis of hybrid nanostructures, containing up-converting lanthanide nanocrystals (doped $NaYF_4$) decorated with semiconducting quantum dot satellites (CdSe) [5]. Solution-casted films of this material reveal remarkable photoconductivity in the near-infrared region, i.e. at sub-band-gap wavelength. These results establish the first application of up-converting nanoparticles in electronic devices.

[1] O. Gidron, A. Dadvand, Y.Sheynin, M. Bendikov, D.F. Perepichka, *Chem. Commun.* 2011, asap (DOI: 10.1039/c0cc04699j)
[2] S. Jeeva, O. Lukoyanova, A. Karapanayiotis, A. Dadvand, F. Rosei, D.F. Perepichka, *Adv. Funct. Mater*. 2010, 20, 1661–1669
[3] J. M. MacLeod, O. Ivasenko, C. Fu, T. Taerum, F. Rosei, D.F.Perepichka, *J. Am. Chem. Soc.* 2009, 131, 16844–16850.
[4] J.A. Lipton-Duffin, J.A. Miwa, M. Kondratenko, F. Cicoira, B. G. Sumpter, V. Meunier, D.F. Perepichka, F. Rosei, *Proc. Nat. Acad. Sci.* USA 2010, 107, 11200–11204.
[5] C. Yan, A. Dadvand, F. Rosei, D. F. Perepichka, *J. Am. Chem. Soc. 2010,* 132, 8868–8869

Dmitrii Perepichka is an Associate Professor in the Department of Chemistry, McGill University (Canada). He received a PhD in chemistry in 1999 from the Institute of the National Academy of Sciences of Ukraine, which was followed by postdoctoral fellowships at Durham University with Martin Bryce and at UCLA with Fred Wudl. His first independent appointment was at INRS-University of Quebec (2003), from where he moved to McGill University in 2005. The research of his group is in a broadly defined area of organic electronic materials, which includes synthesis of polyaromatic molecules and conjugated polymers, their self-assembly and reactions on crystalline surfaces, their interaction with nanomaterials, and their applications in molecular and thin-film electronics. The results of this work was published in over 70 papers (h-index 21) and recognized by several awards such as the DuPont Young Professor (2005) and NSERC Accelerator grants/awards (2003, 2007) and the Feynberg Foundation Scholarship (2009).