
Photovoltaic, light absorption and plasmonic effects in hybrid multilayer systems investigated at a nanometer scale

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The current quest for higher energy-production efficiencies in photovoltaic systems activates various research domains, which include materials science, physics and chemistry, as well as electrical engineering. Beside the fundamental concepts and fabrication methods, which are nowadays established disciplines, our understanding of electrical power generation upon light absorption is almost entirely based on macroscopic investigations realized by averaging large areas of photocurrents. While this is needed for a final device, electron excitations in matter and the required subsequent exciton splitting are inherently nanoscale effects, strongly asking for analyses at the same scale. The combination of local microscopy probes (AFM, C-AFM, hv-AFM...) applied to photovoltaic oxide-based materials grown by pulsed laser deposition (PLD) is therefore essential to understand the behavior at a local scale, before realizing large-scale devices. Little is done in this direction, although some first promising illustrations exist [1], [2].

The main goal in this project is to investigate at the nanometer scale the relationship between the structure and the current-voltage characteristics in hybrid multilayer photovoltaic systems [3] build up from semiconductors (STO, Nb-STO,...), perovskites ferroelectric films (BFO, BFCO,...) and plasmonic metal nanoparticles (Au, Ag, Cu...). These optically active materials have all very good optical properties in both visible and near-infrared spectral range. However, the manner in which the interfacial properties, the defects, the domain polarization and sizes, will precisely impact the overall photovoltaic response still needs a significant experimental work. This thesis aims at investigating these aspects, as the optimization of future photovoltaic systems relies to a very large extent on interface and nanoscopic details. The results will allow optimizing the design of macroscopic solar cells.

Our first experiments and calculations led to promising results significantly surpassing those already reported in the literature [1]. Various optoelectronic effects can be studied this way, with an unprecedented spatial and energetic resolution [4,5,6]. The absorption signal in visible and near infrared regimes can also be monitored in our microscope [5,6]. Hence, a continuous optimization feedback between the growth process of the films and nanoparticles, and the nanoscale opto-electronic properties (band gap values, absorption rates, conversion efficiency, ...) can be realized. In addition, as the force sensibility of an AFM detection scheme goes down to attoNewtons range, our methodology is hence sensitive enough to detect photocurrents without modifying the intrinsic properties of the sample during detection [7,8].

The project includes therefore experimental and theoretical aspects and notions in solid-state physics, optics, electronic effects, and resonant mechanics, are needed. Knowledge of physics and chemistry of materials, oxide films, metal nanoparticles, as well as scanning probe techniques can constitute an important asset for the development of the project.

- [1] M.V. Rastei, F. Gellé, G. Schmerber, A. Quattropani, T. Fix, A. Dinia, A. Slaoui, S. Colis, ACS Appl. Energy Mater. **2**, 8550 (2019). A. Quattropani, A.S. Makhort, M.V. Rastei, G. Versini, G. Schmerber, S. Barre, A. Dinia, A. Slaoui, J.-L. Rehspringer, T. Fix, S. Colis, B. Kundys, Nanoscale. **10**, 13761 (2018).
- [2] J. Alvarez, C. Marchat, A. Morisset, L. Dai, J.-P. Kleider, Raphaël Cabal, P. R. Cabarrocas, Proc. SPIE **11288**, Quantum Sensing and Nano Electronics and Photonics XVII, 112880U (2020).
- [3] Z. Wang, D. Cao, L. Wen, R. Xu, M. Obergfell, Y. Mi, Z. Zhan, N. Nasori, J. Demsar, Y. Lei, Nat. Commun. **7**, 10348, (2016).
- [4] A. Barsella, M. Hurier, M. Pichois, M. Vomir, H. Hasan, L. Mager, B. Donnio, J. L. Gallani, and M. V. Rastei, Phys. Rev. Lett. **125**, 254301 (2020).
- [5] T. Tumkur, M. Hurier, M. Pichois, M. Vomir, B. Donnio, J.L. Gallani, and M.V. Rastei, Phys. Rev. Appl. **11**, 044066 (2019).
- [6] M. Pichois, M. Hurier, M. Vomir, A. Barsella, B. Donnio, J. L. Gallani, and M.V. Rastei, Phys. Rev. Appl. **15**, 034020 (2021).
- [7] M. Alexe, D. Hesse, Nat. Commun. **2**, 256, (2011).
- [8] M.M. Yang, D.J. Kim, M. Alexe. Science **360**, 904, (2018).