

Abstract Submitted  
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**Going beyond DFT for Organic/Titanium Dioxide interfaces<sup>1</sup>**

LEONARDO M. MARION JORGE, MARCELO ALVES-SANTOS, MARÍLIA J. CALDAS, Instituto de Física - Universidade de São Paulo — There is increasing interest in organic/oxide interfaces, particularly for light harvesting and light-emitting devices, and it is important to obtain theoretical information for basic quantities such as the energy-level alignment across the interface. Accurate descriptions of the electronic structure of the composite system, as e.g. [1], are however scarce. The method used should give reliable results for both organic and oxide materials, to guarantee a good description of the hybrid system. In this work we have explored different DFT functionals (PZ-LDA, and those that include a fraction of Exact-Exchange as PBE0, HSE and B3LYP [2]) and compared the results with those obtained by Many-Body Perturbation theory with the GW approximation[3]. We have chosen as prototype systems TiO<sub>2</sub>, both bulk crystal and model surface, and Thiophene. We have found that none of the used DFT schemes give optimal results for both organic and inorganic systems at the same time, so moving beyond DFT is mandatory.

[1] C.D. Valentin et.al., Phys. Rev. Lett. 97, 166803 (2006)

[2] J.P. Perdew et.al., J. Chem. Phys. 105, 9982 (1996); J. Heyd et.al., J. Chem. Phys. 118, 8207 (2003); P.J. Stephens et.al., J. Phys. Chem. 98, 11623 (1994)

[3] A. Marini et.al., Comp. Phys. Comm. 180, 1392 (2009)

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Leonardo M. Marion Jorge  
Instituto de Física - Universidade de São Paulo

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