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Electrodeposited ZnO Nanowires as Photoelectrode in Solid-State Organic Dye-Sensitized Solar Cells

Hervé Muguerra§, Gaëlle Berthoux§, Wan Zaireen Nisa Yahya§, Yann Kervella§,
Valentina Ivanova#, Johann Bouclé†*, Renaud Demadrille§*

§INAC/SPrAM (UMR 5819 CEA-CNRS-Univ. J. Fourier-Grenoble), LEMOH,
17 Rue des Martyrs, 38054 Grenoble Cedex 9, France.
#CEA-Leti, MINATEC Campus
17 rue des Martyrs, 38054 Grenoble Cedex 9, France.
†XLIM UMR 7252, Université de Limoges/CNRS,
123 Avenue Albert Thomas, 87060 Limoges Cedex, France
*Corresponding Author: Dr. R. Demadrille, Phone number: +33(0)438784484, Fax number: +33(0)438785145, E-mail: renaud.demadrille@cea.fr.

Dr. R. Johann Bouclé, Phone number: +33(0)587506762, Fax number: +33(0)555457649, E-mail:johann.boucle@unilim.fr.
Figure ESI. Frontier orbitals (HOMO and LUMO) of PK1 optimized with DFT at the B3LYP/TZ2P level, energy levels estimated from DFT (black) and from the oxidation potential and reduction potential determined by cyclic voltammetry experiments (blue). Cyclic voltammetry measurements were carried out in dichloromethane solution (10^{-3} M) at a scan rate of 20 mV s^{-1}. The redox potential of Fc/Fc^+ which has an absolute energy level of -4.8 eV relative to the vacuum level for calibration is located at +0.23 V in 0.1 M TBAPF6/anhydrous CH₂Cl₂ solution.

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