

ESI

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

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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 $+0.23 \text{ V}$ in $0.1 \text{ M TBAPF}_6/\text{anhydrous } \text{CH}_2\text{Cl}_2$ solution.

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