

Correction to Elucidating Band-Selective Sensitization in Iron(II) Polypyridine-TiO₂ Assemblies

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Supporting Information

Page 8627. We have recently found that our previously published calculated interfacial electron transfer (IET) rates for the [Fe(bpy-dca)₂(CN)₂]-TiO₂ system in “bpy perpendicular” orientation were not converged with respect to the simulation cell size (supercell of lattice dimensions $a = 30.49$ Å, $b = 31.46$ Å, and $c = 26.00$ Å). Additionally, the characteristic IET time from LUMO+1 of this sensitizer in the “bpy parallel” orientation with a bidentate carboxylic acid attachment was incorrectly plotted as 1.67×10^2 fs when it was in fact 1.67×10^5 fs. These characteristic IET times are shown in Figure 13 of the original manuscript.

The quantum dynamics simulations were repeated for all linker models of the [Fe(bpy-dca)₂(CN)₂]-TiO₂ system with a supercell of new lattice dimensions $a = 30.49$ Å, $b = 31.46$ Å, and $c = 34.00$ Å. The corrected characteristic IET times for the [Fe(bpy-dca)₂(CN)₂]-TiO₂ system are shown in the corrected Figure 13.

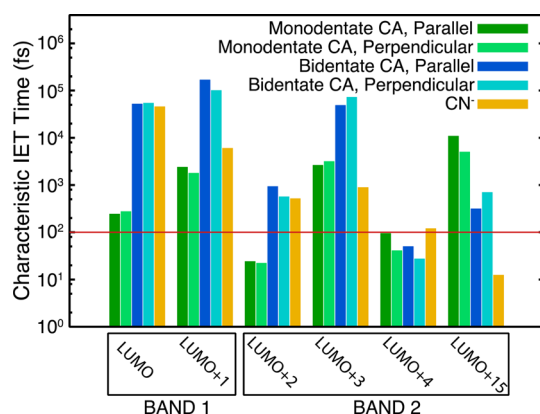


Figure 13. Characteristic IET times for relevant particle states of [Fe(bpy-dca)₂(CN)₂] attached to the anatase (101) slab by monodentate carboxylic acid (in both the “bpy parallel” and “bpy perpendicular” orientations), bidentate carboxylic acid (in both the “bpy parallel” and “bpy perpendicular” orientations), and cyanide anchoring groups, determined by exponential fitting.

The corrections described here do not change or invalidate any of the conclusions reported in the original publication.

■ ASSOCIATED CONTENT

Supporting Information

Plots of the survival probability as well as characteristic IET times determined by single and biexponential fitting. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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