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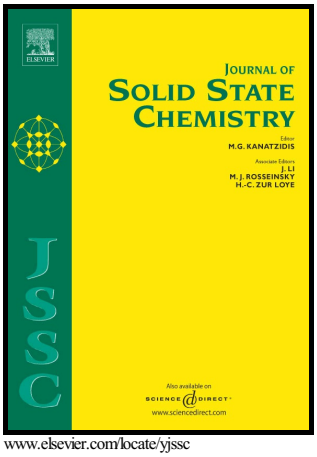

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Configurations, band structures and photocurrent responses of 4-(4-oxopyridin-1(4H)-yl)phthalic acid and its metal-organic frameworks

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Abstract

4-(4-oxopyridin-1(4H)-yl)phthalic acid (**H_2L**) and three **H_2L**-based metal-organic frameworks (MOFs) formulated as ZnL(DPE)(H_2O)·H_2O (DPE = (*E*)- 1, 2- di(pyridine -4-yl)ethene) (**1**), CdL(H_2O)$_2$ (**2**) and CdL (**3**) were synthesized and structurally characterized by single-crystal X-ray diffraction. The free **H_2L** ligand shows an *enol*-form and the **L^{2-}** ligand in the three MOFs exists as the *keto*-form. Density functional theory (DFT) calculations indicate **H_2L** and the three MOFs possess different band structures. Due to the existence of the N-donor, **DPE** in MOF **1**, the conduction band (CB) minimum and band gap of MOF **1** are much lower than those of **H_2L**. And MOF **1** yielded much larger photocurrent density than **H_2L** upon visible light illumination. Electrochemical impedance spectroscopy (EIS) shows the interfacial charge transfer impedance in the presence of MOF **1** is lower than that in the presence of **H_2L.** The hydrous MOF **2** and the

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