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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<sub>2</sub>L**) and three **H<sub>2</sub>L**-based metal-organic frameworks (MOFs) formulated as ZnL(DPE)(H<sub>2</sub>O)·H<sub>2</sub>O (DPE = (E)- 1, 2- di(pyridine -4-yl)ethene) (**1**), CdL(H<sub>2</sub>O)<sub>2</sub> (**2**) and CdL (**3**) were synthesized and structurally characterized by single-crystal X-ray diffraction. The free **H<sub>2</sub>L** ligand shows an *enol*-form and the **L<sup>2-</sup>** ligand in the three MOFs exists as the *keto*-form. Density functional theory (DFT) calculations indicate **H<sub>2</sub>L** 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<sub>2</sub>L**. And MOF **1** yielded much larger photocurrent density than **H<sub>2</sub>L** 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<sub>2</sub>L**. The hydrous MOF **2** and the

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