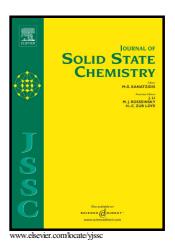
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Configurations, band structures and photocurrent responses of 4-(4-oxopyridin-1(4H)-yl)phthalic acid and its metal-organic frameworks

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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

 $\hbox{$4$-(4-oxopyridin-1(4H)-yl)phthalic acid (H_2L) and three H_2L-based metal-organic frameworks}$

(MOFs) formulated as $ZnL(DPE)(H_2O) \cdot H_2O$ (DPE = (E)- 1, 2- di(pyridine -4-yl)ethene) (1),

CdL(H₂O)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 H₂L. 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 H₂L. The hydrous MOF 2 and the

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