## Supporting Information

# A Rational Design for Dye-Sensitizer: Density Functional Theory Study on the Electronic Absorption Spectra of Organoimido-Substituted Hexamolybdates

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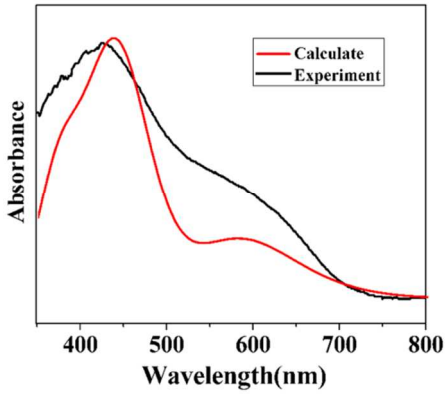


**Figure.** Experimental and calculated absorption spectra of system **1**.

The comparison between the calculated and experimental absorption spectra of system **1** is important to ensure the theoretical method is accurate in predicting the electronic absorption spectra of designed systems. The Figure shows that the calculated absorption spectra (red line) of system **1** by SAOP is in good agreement with the experimental result of α type crystal (black line) and the difference of maximum absorption band between them is only 13 nm.[22] Therefore, the credible electronic absorption spectra of systems can be obtained by SAOP.