Supporting Information

Title: Microwave and ultrasonic assisted synthesis 2D La-based MOFs nanosheets by coordinative unsaturation degree to boost phosphate adsorption.

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1. Materials and methods

1.1 Characterizations and Density functional theory calculation

The apparent total pore volume and Brunauer-Emmett-Teller (BET) surface area (SBET) were identified by the test of N2 adsorption-desorption on pore structural analyzer (TriStarII3020). And the powder X-ray diffraction (XRD, Rigaku, Japan) with patterns Cu-Kα radiation (250 mA, 40kV) scanned the prepared material to determine crystalline structure and composition (2θ: 5º-50º). The microstructures of samples were collected on scanning electron microscopy (SEM, FEI, USA). The thickness of the sample is characterized by atomic force microscope(AFM). Transmission electron microscope (TEM) imaging were obtained by transmission electron microscope (FEI, Tecnai-G20). Zeta potentials were determined by using zeta potential analyzer (ZS-90, Malvern). A FTIR (Nicolet IS 10) was employed to collect the FTIR spectra with KBr pellets in the range of 4000-400 cm-1. Thermogravimetric analyses (TGA, NETZSCH STA 449F3) were conducted by heating the product from room temperature to 1000 ℃ in N2 atmosphere. The surface chemical states of products were examined using XPS (PHI5000, ULVAC-PHI Inc., Japan, Al Kα).

DFT simulation calculation was performed by the CASTEP module in MaterialsStudio2019. Further, GGA-PBEsol was selected to achieve the function of exchange interaction. The criteria about structure and energy convergence as follows: the energy convergence criterion was 1.0×10^{-5}eV/atom, the maximum displacement tolerance was 0.001Å. Meanwhile, 0.05eV/Å was set as the maximum force tolerance. In addition, the convergence error on self-consistent field (SCF) cannot exceed 1.0×10^{-6} eV/atom.

2. DFT calculation results

DFT calculation results are listed in the data document.