Electronic Supplementary Material (ESI) for RSC Advances.

Highly Selective and Efficient Adsorption Dyes Self-assembled by 3D Hierarchical Architecture of Molybdenum Oxide

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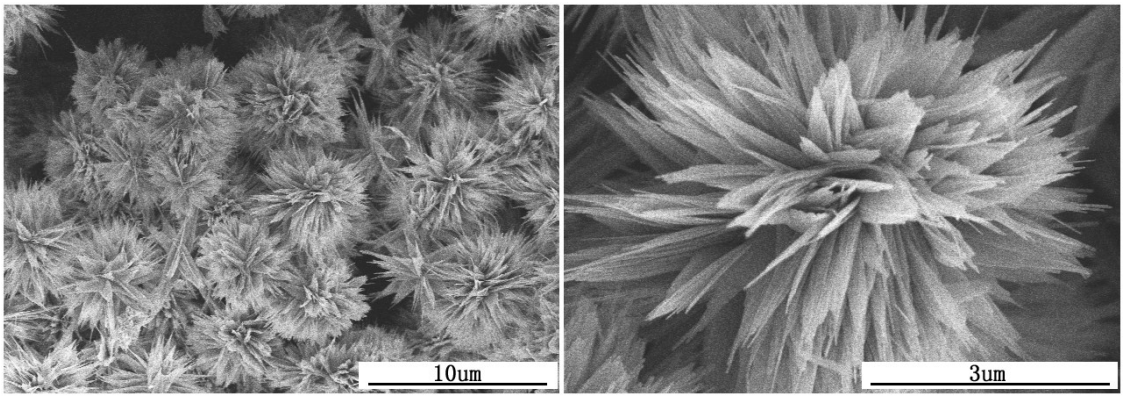


Figure S1 Low-magnification (a) and high-magnification (b) SEM images of the MoO_3 flower-like microspheres calcined at 250 ^oC

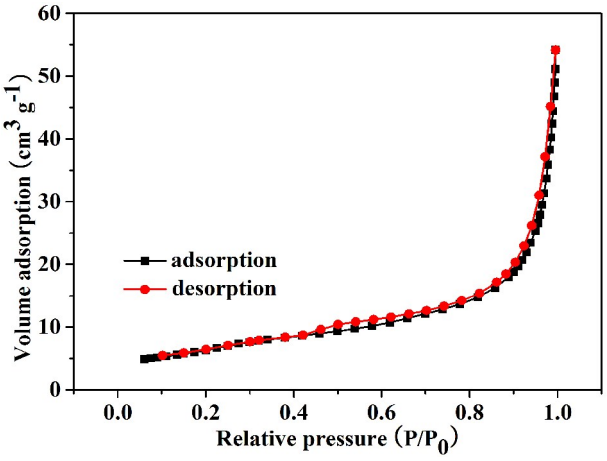


Figure S2 Nitrogen adsorption-desorption isotherms of nanoflower-like α-MoO_3

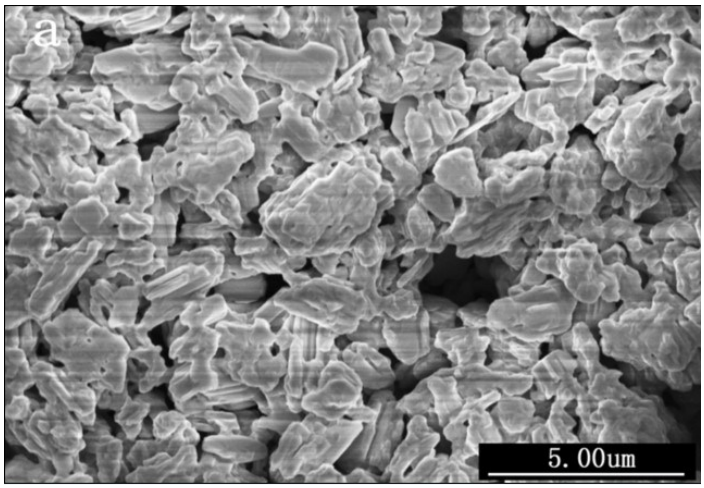


Figure S3 Typical SEM image of the commercial α-MoO_3

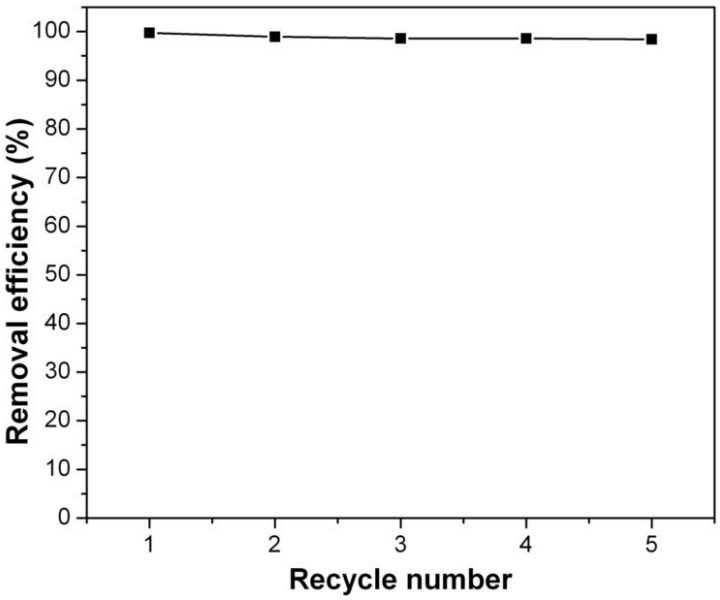


Figure S4 The correlation between the removal efficiency of RhB and regeneration recycle numbers.

Figure S5 The photographs of MoO_3 microspheres before (a) and after (b) adsorption of RhB, and ethanol washed sample (c) after adsorption.

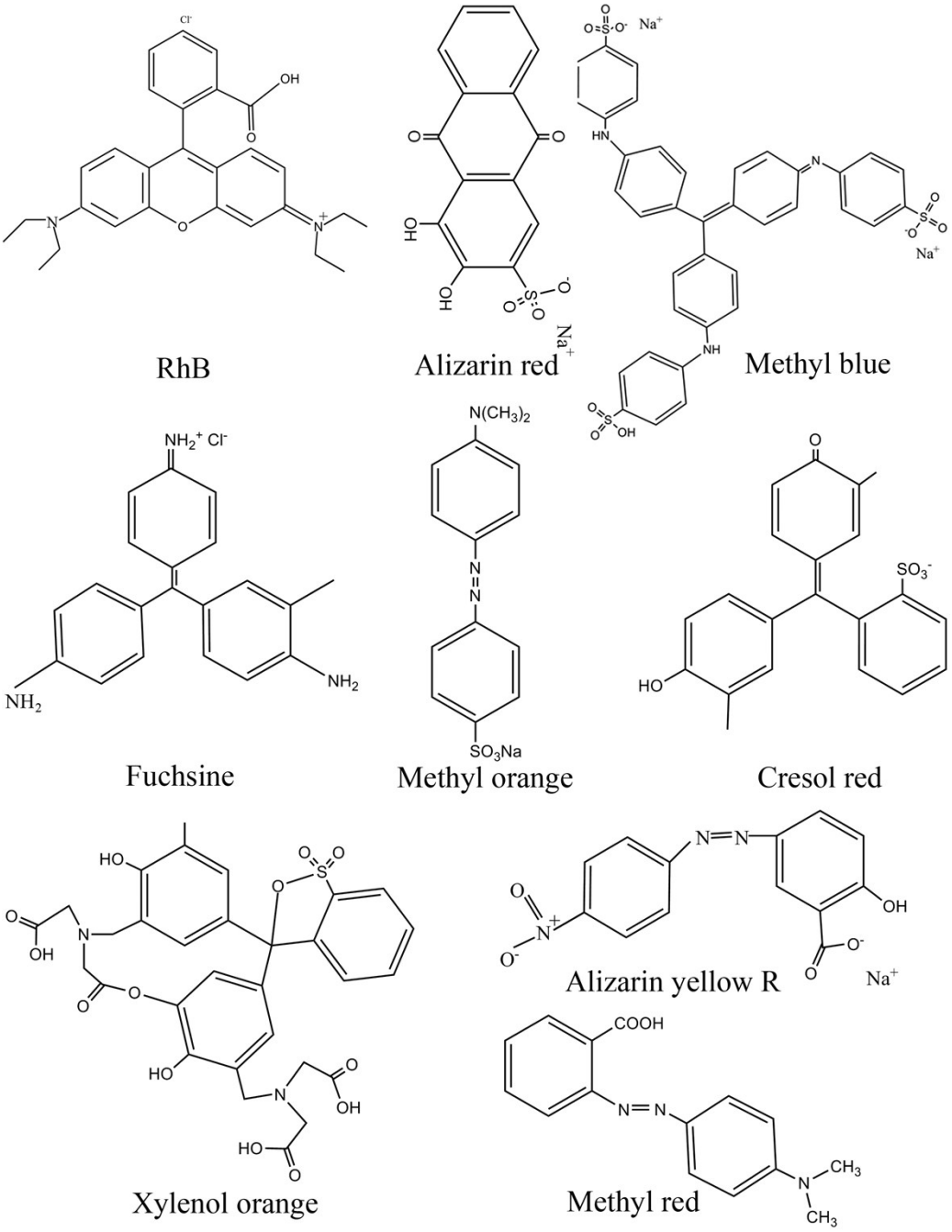


Figure S6 The molecular structure diagrams of the nine adsorbed molecules

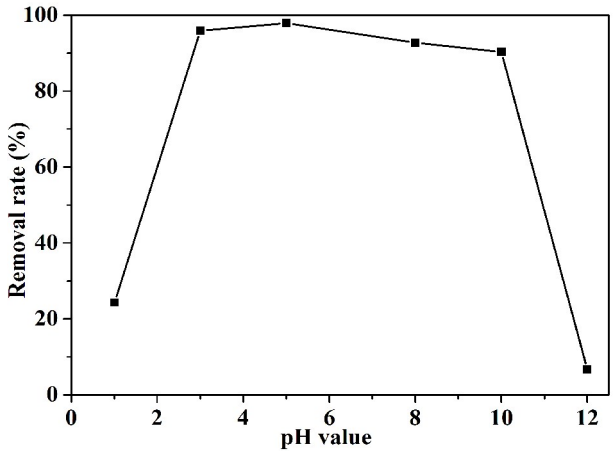
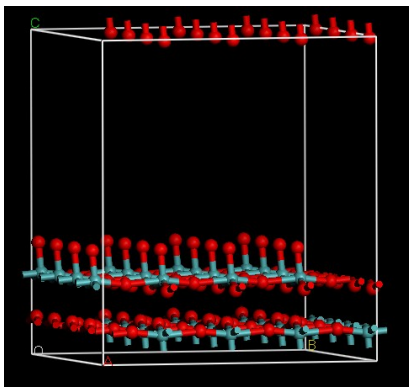
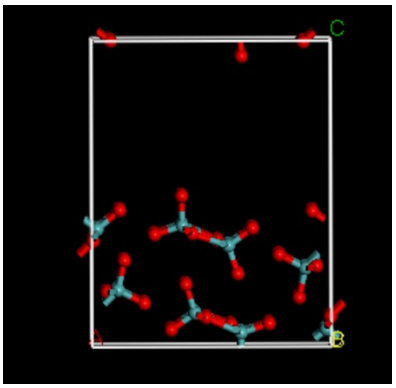


Figure S7 pH values effect on adsorption performance

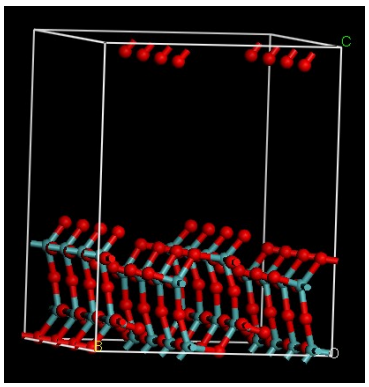
Three important surface structures of α-MoO_3, e.g. (010), (100), and (001) crystalline plane, were taken into account in the calculations. Their optimized geometry structures were shown in Figure S8. The three surface structures have identical type and number of atoms and hence should be isomers. The total energies (Figure S8) for the three structures are in the order (010) > (100) > (001) (the relative energies of them is 0 eV, 7.8 eV and 12.25 eV), which is in accordance with their sequence of surface areas.



(010) E_{total}=−1054.16



(100) E_{total}=−1046.34

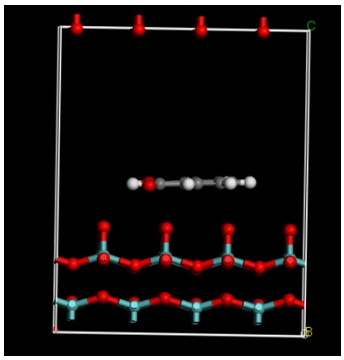
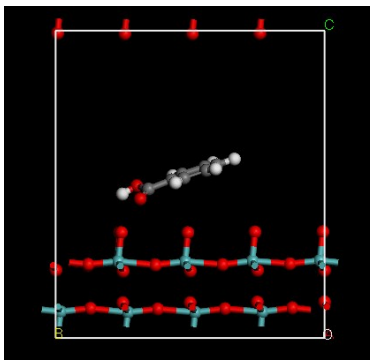
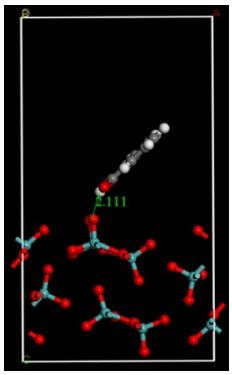
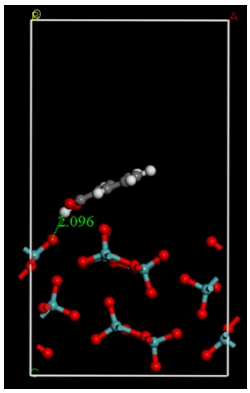
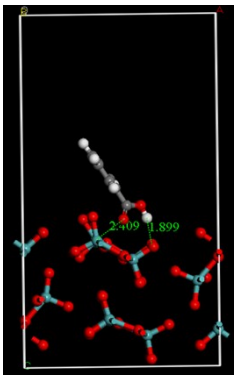


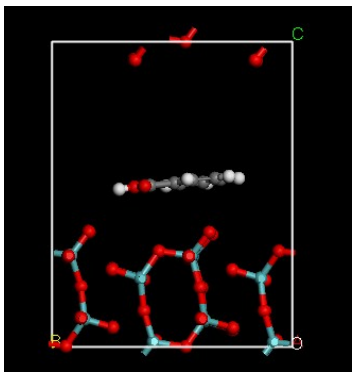
(001) E_{total}=−1041.90

Figure S8 The optimized structures for (010), (100), and (001) surfaces of α-MoO_3 associated with their total energies in eV.

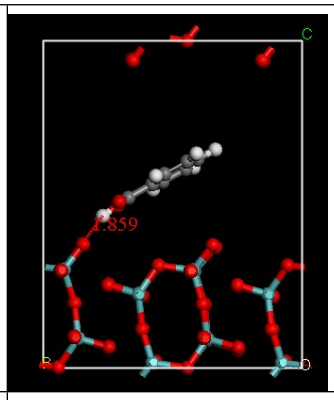
To clarify which crystalline plane ((010), (100), and (001)) of α-MoO_3 has the most strong adsorption ability to organic molecules, C_6H_5COOH was selected as a test molecule. Taking into account various unsaturated sites on the surfaces of α-MoO_3,

we obtained possible adsorption structures for the three surfaces, which were shown in Figure S9 associated with their binding energies. As seen in Figure S9, the adsorption ability of C_6H_5COOH to the surfaces of α-MoO_3 should be in the order (010) < (100) < (001), just opposite to their stability order. It is not surprising that the (010) plane has the weakest adsorption to C_6H_5COOH because the terminal oxygen atoms of (010) surface prohibit the effective interaction between Mo and O atoms of C_6H_5COOH, which is the major contribution to the binding energy. With respect to (100) and (001) plane, although both of them have similar adsorption sites, the short Mo(α-MoO_3)-O(C_6H_5COOH) distance (shown in Figure S9) can be responsible for the strongest adsorption of (001) surface to C_6H_5COOH molecule.

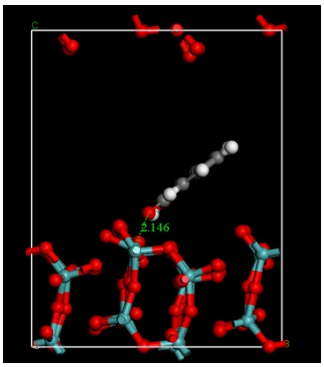
		
(010)-1 $E_{binding}$=−0.0462	(010)-2 $E_{binding}$=−0.0299	
		
(100)-1 $E_{binding}$=−0.157	(100)-2 $E_{binding}$=−0.0578	(100)-3 $E_{binding}$=−0.701



(001)-1 $E_{binding}$=−0.0716



(001)-2 $E_{binding}$=−0.1429



(001)-3 $E_{binding}$=−1.619

Figure S9 Adsorption structures of C_6H_5COOH onto (010), (100), and (001) surfaces of α-MoO_3 associated with their binding energies in eV.