

Electronic Supplementary Material (ESI) for CrystEngComm

## **Cu<sup>II</sup>-based metal-organic nanoballs for very rapid adsorption of dyes and iodine**

Eder Amayuelas,<sup>a</sup> Arkaitz Fidalgo-Marijuán,<sup>a</sup> Begoña Bazán,<sup>a,b</sup> Miren-Karmele Urriaga,<sup>a</sup> Gotzone Barandika,<sup>\*,c</sup> and María-Isabel Arriortua.<sup>a,b</sup>

<sup>a</sup>*Departamento de Mineralogía y Petrología, Universidad del País Vasco (UPV/EHU), Barrio Sarriena s/n, 48940 Leioa, Bizkaia.*

<sup>b</sup>*BCMaterials, Basque Center for Materials, Applications and Nanostructures, Parque Tecnológico de Zamudio, Ibaizabal Bidea, Edificio 500-Planta 1, 48160 Derio, Bizkaia.*

<sup>c</sup>*Departamento de Química Inorgánica Universidad del País Vasco (UPV/EHU), Barrio Sarriena s/n, 48940 Leioa, Bizkaia.*

Fig. S1 Thermodiffraction of <b>MOP@Ei2-1</b> .	2
Fig. S2 IR spectra of <b>MOP@Ei2-1</b> (blue) and <b>αMOP@Ei2-1</b> (red).	2
Fig. S3 UV-Vis diffuse reflectance of <b>MOP@Ei2-1</b> and <b>αMOP@Ei2-1</b> .	3
Fig. S4 IR of <b>MOP@Ei2-1</b> (red) and samples of <b>MOP@Ei2-1</b> after 3 days dispersed in boiling water (green) and in boiling EtOH (blue).	3
Fig. S5 Lewis Structures of dyes used.	4
Fig. S6 IR of <b>αMOP@Ei2-1</b> and samples of <b>αMOP@Ei2-1</b> loaded with <b>MB</b> , <b>CR</b> and <b>DY</b> .	4
Fig. S7-S12 (a) UV-Vis spectrum of dyes and iodine and (b) calibration line performed with solutions of different concentrations.	5, 6
Fig. S13 View of the removed quantities of dyes and iodine after 7 days.	7
Fig. S14 Color changes of <b>αMOP@Ei2-1</b> after adsorption experiments.	7
Fig. S15 First order kinetics adjustment for (a) <b>CR</b> , (b) <b>MB</b> , (c) <b>DY</b> and (d) <b>I<sub>2</sub></b> .	8
Table S1 Molecular dimensions (Å) of dyes.	8

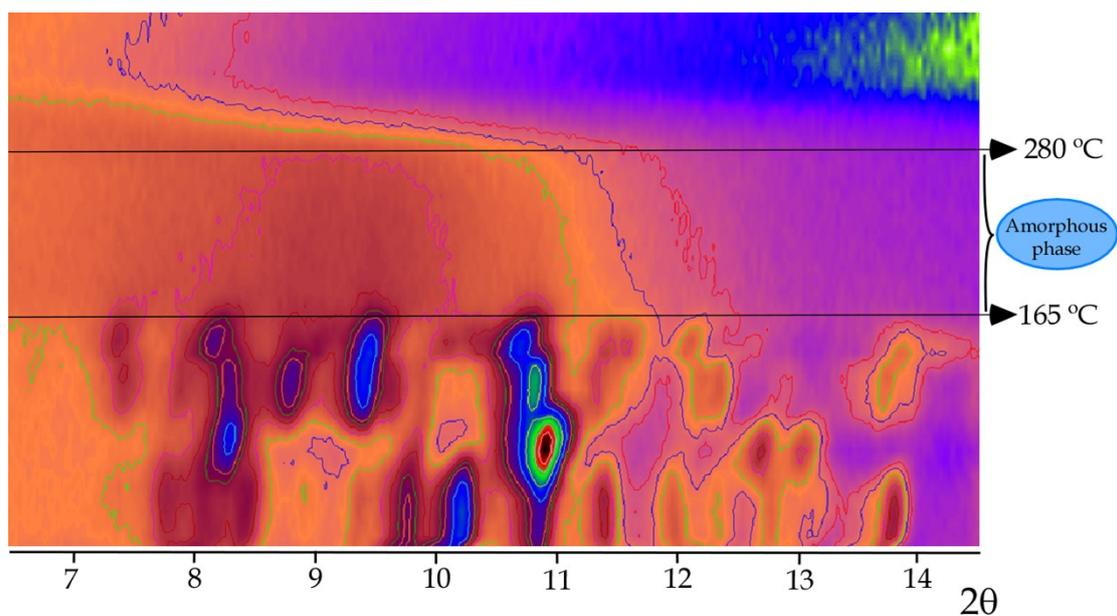


Fig. S1 Thermodiffractometry of MOP@Ei2-1.

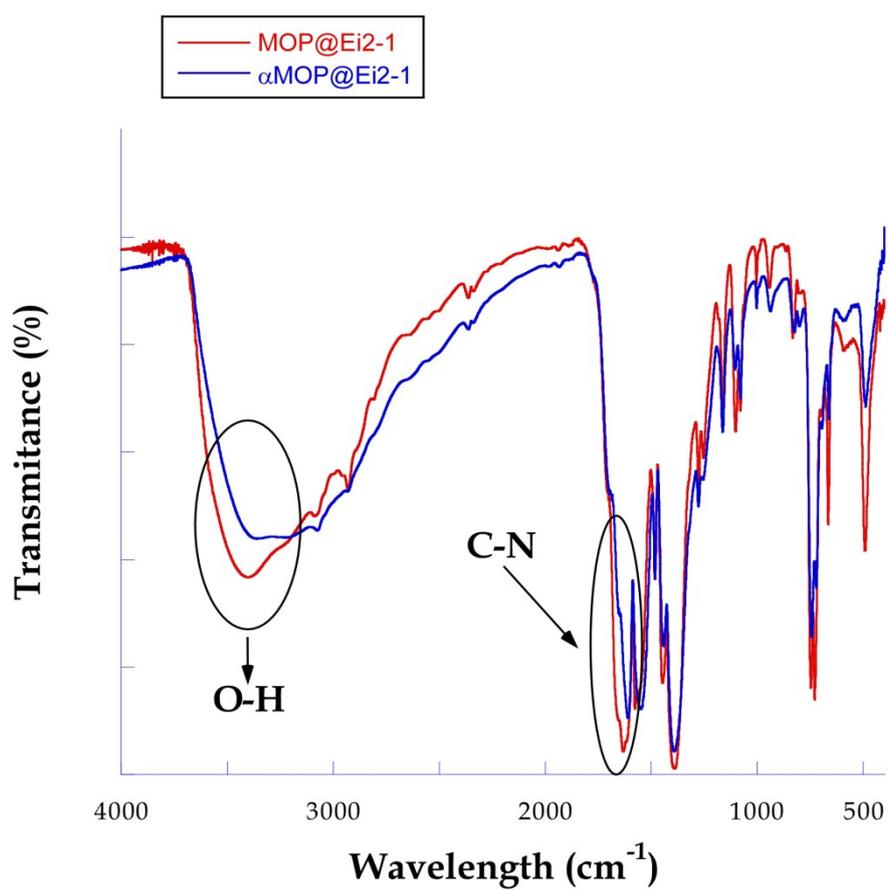
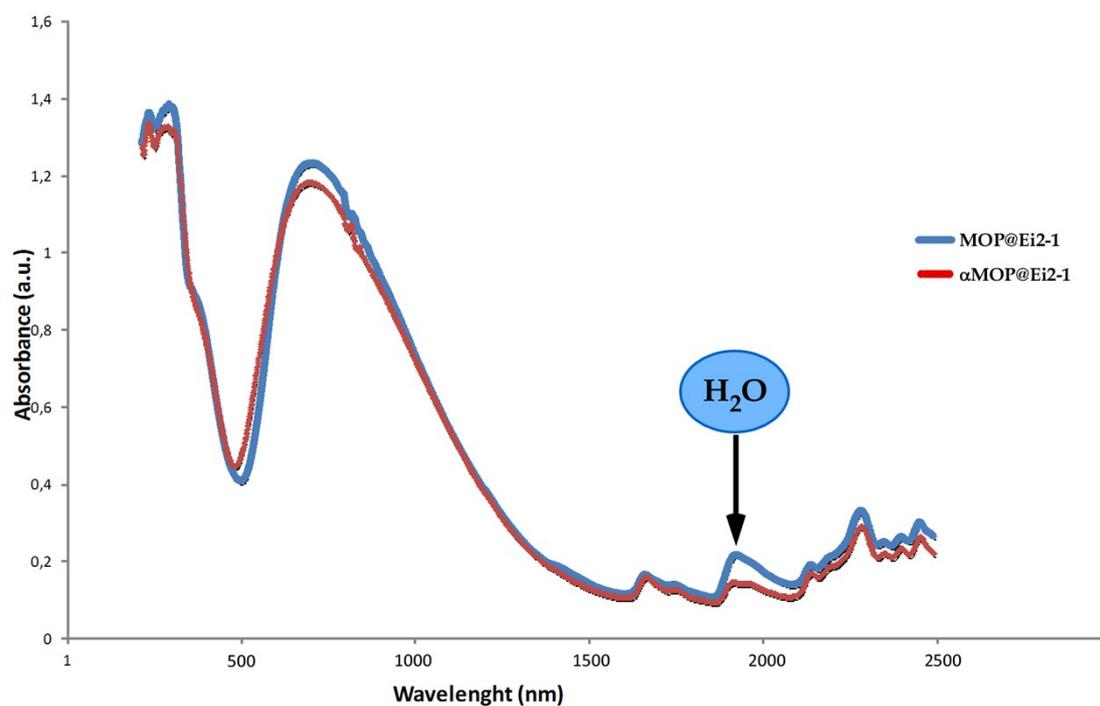
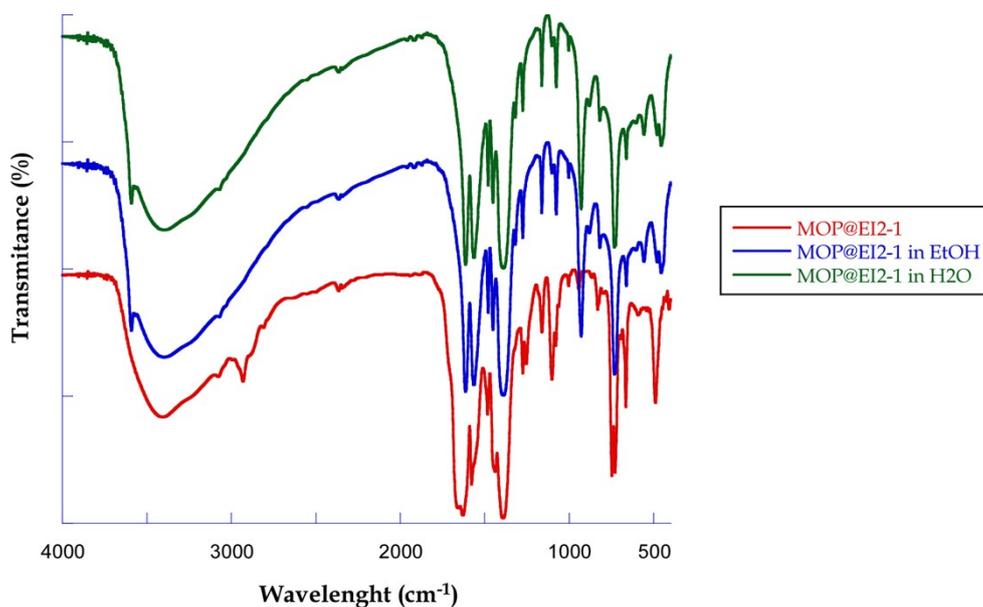


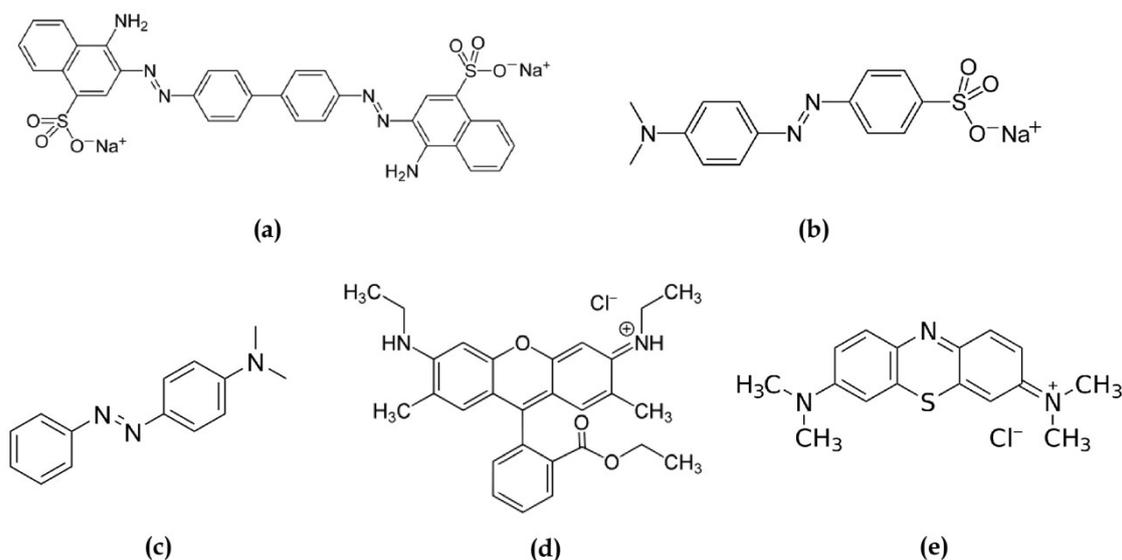
Fig. S2 IR spectra of MOP@Ei2-1 (blue) and  $\alpha$ MOP@Ei2-1 (red).



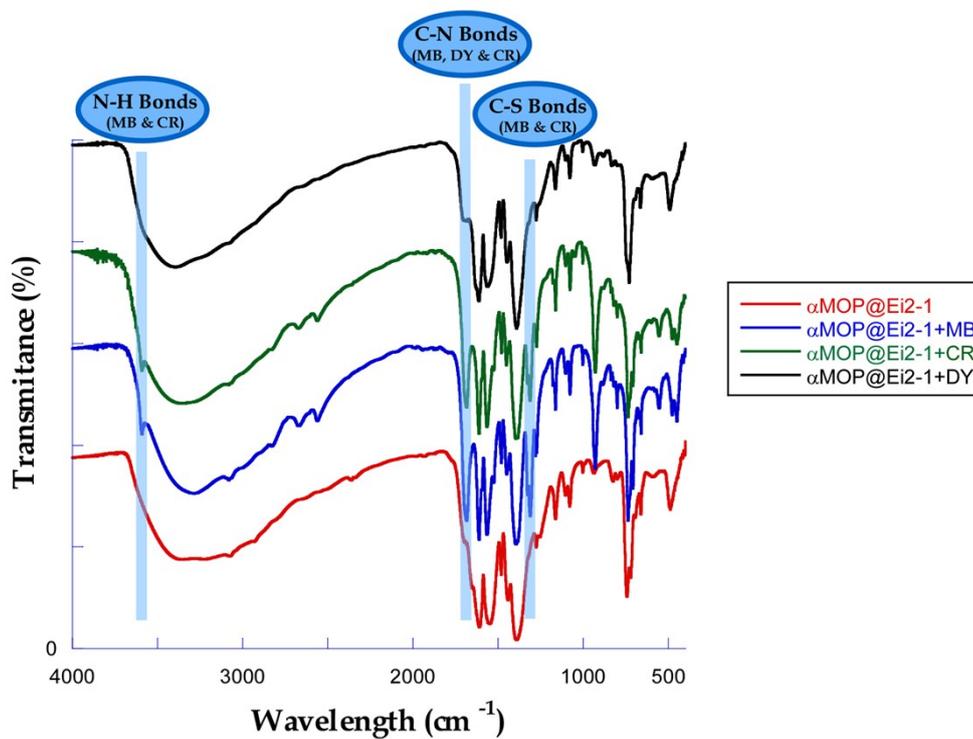
**Fig. S3** UV-Vis diffuse reflectance of **MOP@Ei2-1** and **αMOP@Ei2-1**.



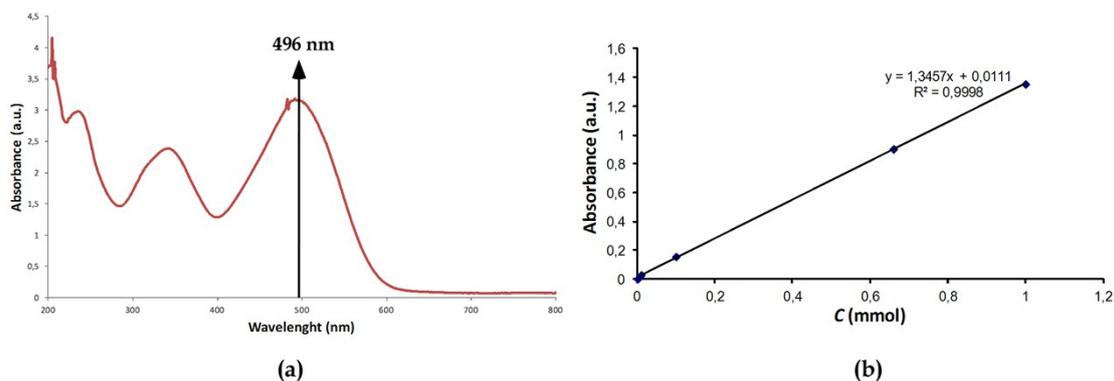
**Fig. S4** IR of **MOP@Ei2-1** (red) and samples of **MOP@Ei2-1** after 3 days dispersed in boiling water (green) and in boiling EtOH (blue).



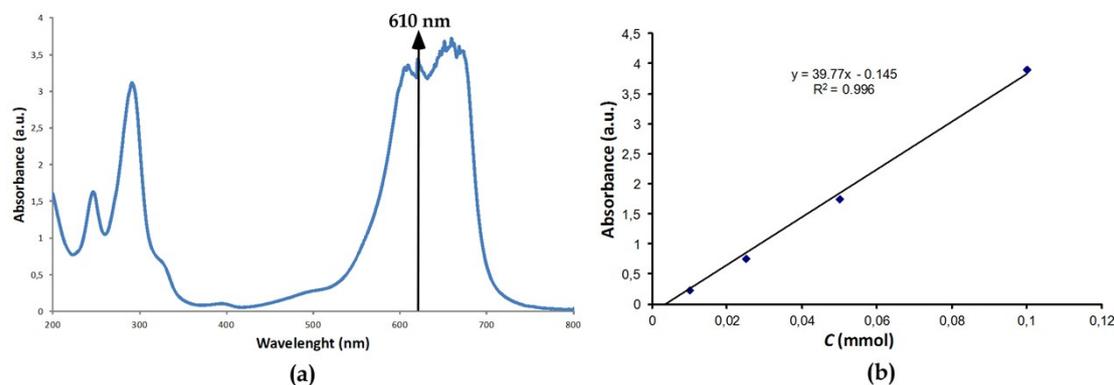
**Fig. S5** Lewis Structures of dyes used: (a) Congo Red (**CR**), (b) Methyl Orange (**MO**), (c) Dimethyl Yellow (**DY**), (d) Rhodamine 6G (**R6G**) and (e) Methylene Blue (**MB**).



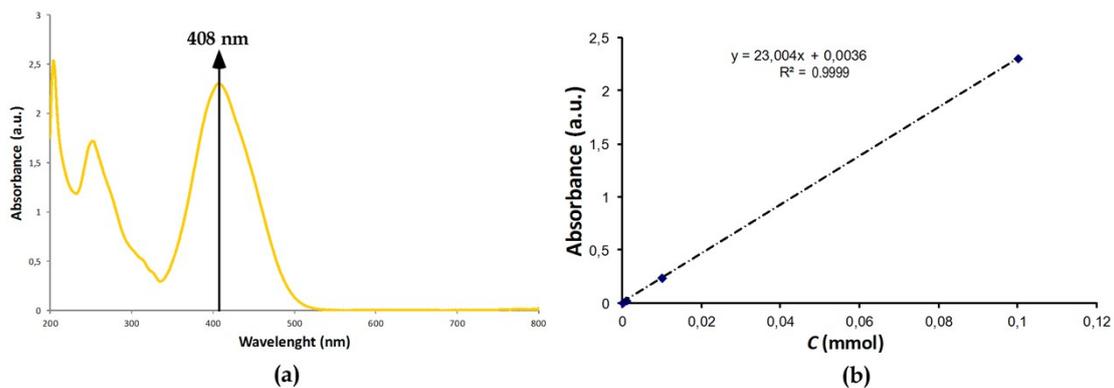
**Fig. S6** IR of  $\alpha$ MOP@Ei2-1 and samples of  $\alpha$ MOP@Ei2-1 loaded with MB, CR and DY.



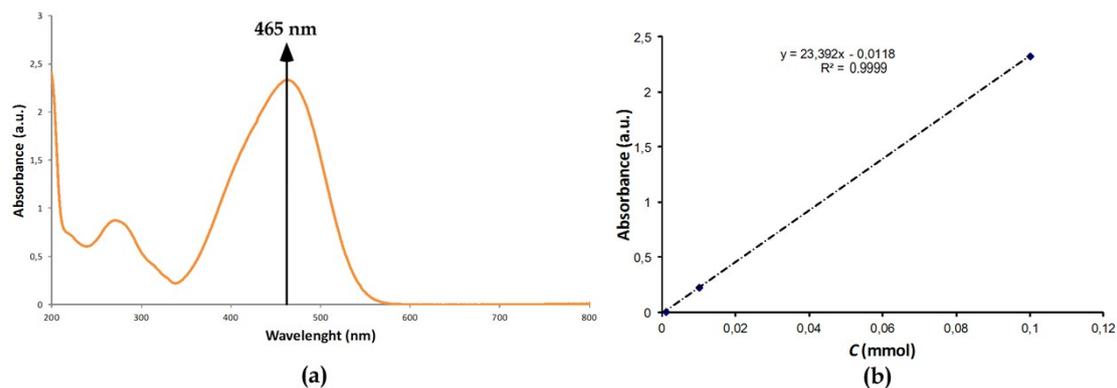
**Fig. S7** (a) CR UV-Vis spectrum and (b) calibration line performed with solutions of different concentrations of CR ( $1 \times 10^{-4}$  M,  $1 \times 10^{-5}$  M,  $1 \times 10^{-6}$  M and  $1 \times 10^{-7}$  M). UV-Vis measurements for CR were performed at 496 nm.



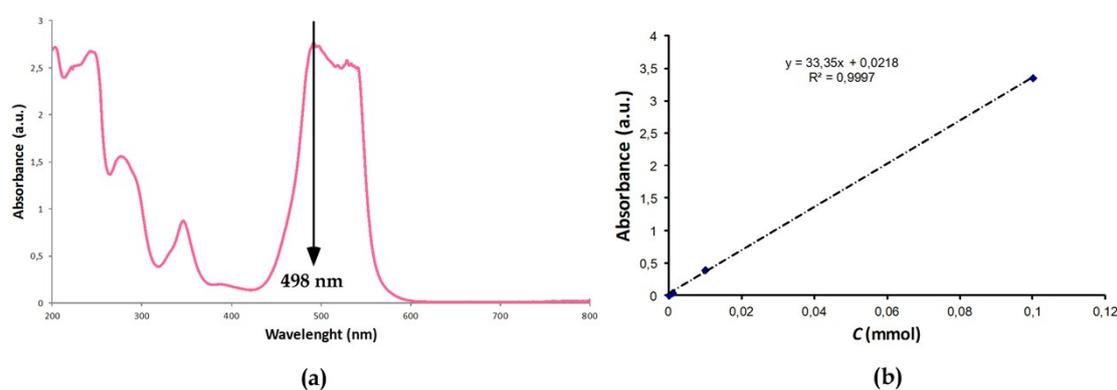
**Fig. S8** (a) MB UV-Vis spectrum and (b) calibration line performed with solutions of different concentrations of MB ( $1 \times 10^{-4}$  M,  $1 \times 10^{-5}$  M,  $1 \times 10^{-6}$  M and  $1 \times 10^{-7}$  M). UV-Vis test for MB were measured at 610 nm.



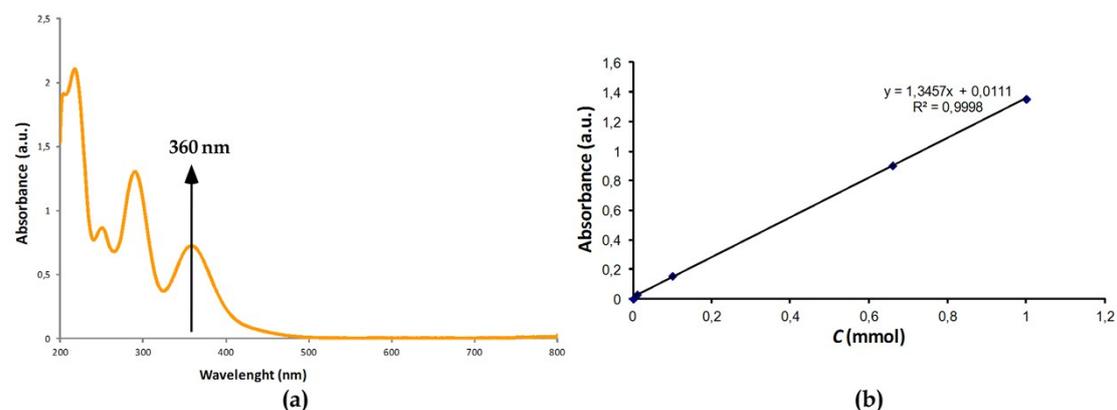
**Fig. S9** (a) DY UV-Vis spectrum and (b) calibration line performed with solutions of different concentrations of DY ( $1 \times 10^{-4}$  M,  $1 \times 10^{-5}$  M,  $1 \times 10^{-6}$  M and  $1 \times 10^{-7}$  M). UV-Vis test for DY were measured at 408 nm.



**Fig. S10** (a) **MO** UV-Vis spectrum and (b) calibration line performed with solutions of different concentrations of **MO** ( $1 \times 10^{-4}$  M,  $1 \times 10^{-5}$  M,  $1 \times 10^{-6}$  M and  $1 \times 10^{-7}$  M). UV-Vis test for **MO** were measured at 465 nm.



**Fig. S11** (a) **R6G** UV-Vis spectrum and (b) calibration line performed with solutions of different concentrations of **R6G** ( $1 \times 10^{-4}$  M,  $1 \times 10^{-5}$  M,  $1 \times 10^{-6}$  M and  $1 \times 10^{-7}$  M). UV-Vis test for **R6G** were measured at 498 nm.



**Fig. S12** (a)  $I_2$  UV-Vis spectrum and (b) calibration line performed with solutions of different concentrations of  $I_2$  ( $1 \times 10^{-3}$  M,  $1 \times 10^{-4}$  M,  $1 \times 10^{-5}$  M,  $1 \times 10^{-6}$  M and  $1 \times 10^{-7}$  M). UV-Vis test for  $I_2$  were measured at 360 nm.

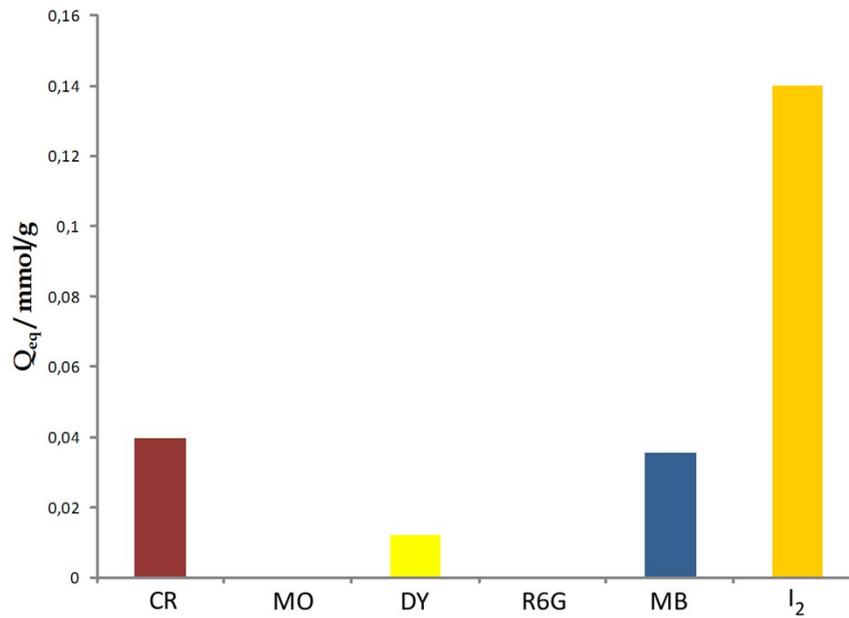


Fig. S13 View of the removed quantities of dyes and iodine after 7 days.

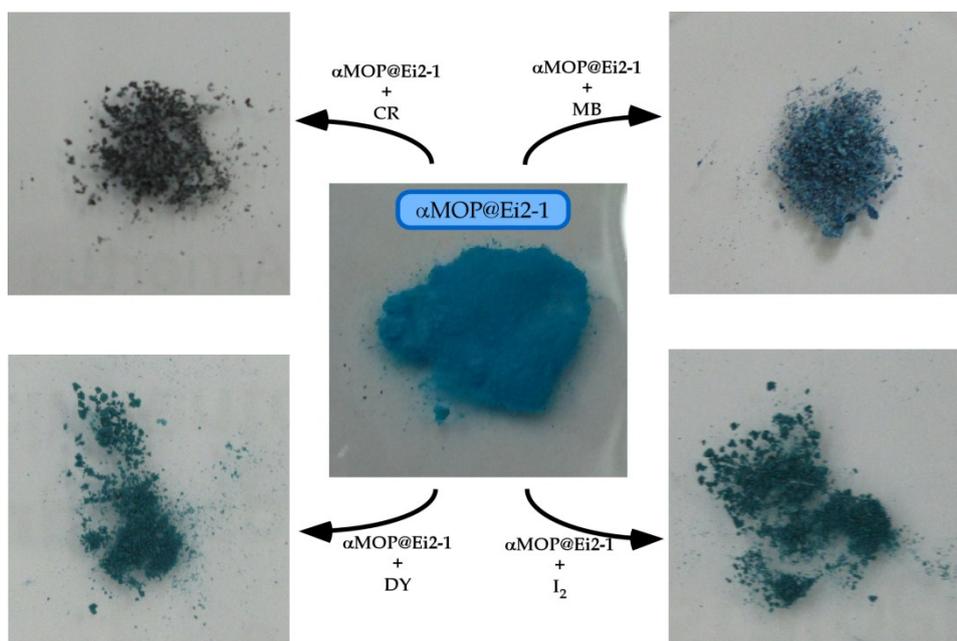
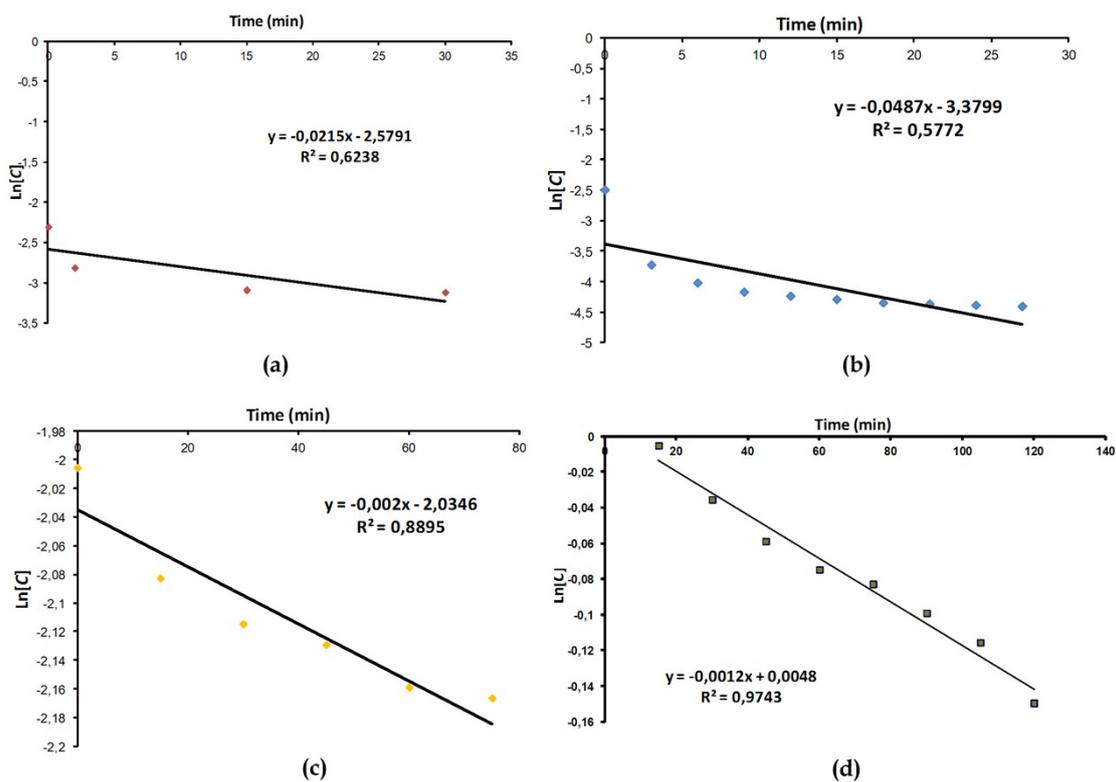


Fig. S14 Color changes of  $\alpha$ MOP@Ei2-1 after adsorption experiments.



**Fig. S15** First order kinetics adjustment for (a) **CR**, (b) **MB**, (c) **DY** and (d) **I<sub>2</sub>**. First range of adsorption was taken for the adjustment, until the saturation of **αMOP@Ei2-1** begins.

**Table S1** Molecular dimensions (Å) of dyes.

	<b>MB</b>	<b>CR</b>	<b>DY</b>	<b>MO</b>	<b>R6G</b>
<b>x (width)</b>	4.59	5.38	4.5	5.31	10.89
<b>y (height)</b>	8.01	7.9	6.0	7.25	15.72
<b>z (length)</b>	16.75	25.1	15.1	17.39	15.79