Empowering adsorption and photocatalytic degradation of ciprofloxacin

on BiOI composites:

A materials-by-design investigation

Sepideh G. Khasevani^a, Dariush Nikjoo^a, Cécile Chaxel^a, Kentaro Umeki^a, Shokat Sarmad^b,

Jyri-Pekka Mikkola^{b, c}, Isabella Concina^{a*}

^aLuleå University of Technology, Department of Engineering Sciences and Mathematics,

98187 Luleå, Sweden

^bWallenberg Wood Science Center, Department of Chemistry Technical Chemistry, Department of Chemistry, Chemical-Biological Centre, Umeå University, SE-90871 Umeå, Sweden

^cIndustrial Chemistry & Reaction Engineering, Johan Gadolin Process Chemistry Centre,

Åbo Akademi University, FI-20500 Åbo-Turku, Finland

* Corresponding author: isabella.concina@ltu.se

Supplementary Information



Figure S 1. CIP adsorption under dark vs. F-BC content for the ternary composites.



Figure S 2. Fitting according to a pseudo-second order model of the absorption process supported by the materials under investigation. Markers are experimental points, lines are fitting equations. Integrated equation: $q_t = \frac{q_e^2 k_2 t}{1 + q_e k_2 t}$.

Material	R ²	Slope (g mg ⁻¹)	Intercept (g mg ⁻¹ min)
BiOI	0.98599	0.02544 ± 0.00152	1.022
BiOI/MOF 10%	0.98690	0.01467 ± 0.06582	0.7698
BiOI/MOF 20%	0.99337	0.01446 ± 0.00059146	0.9936
BiOI/MOF 30%	0.98821	0.0136 ± 0.00074292	0.6739
BiOI/MOF 50%	0.99700	0.01368 ± 0.00037544	1.938
BiOI/MOF/F-BC 5%	0.98787	0.01415 ±0.00078370	0.9787
BiOI/MOF/F-BC 10%	0.99944	0.0141 ± 0.00053052	1.721
BiOI/MOF/F-BC 20%	0.99580	$0.01309 \pm 0.0004.2494$	0.9751

Table S 1. Parameters of the fitting of the adsorption process for the materials under investigation.



Figure S 3. CIP degradation under simulated solar light catalyzed by the binary composites vs. MOF content. Markers are experimental points; the dashed line is the exponential fit of the data.



Figure S 4. Recyclability runs for the ternary composite BiOI/MOF/F-BC 10%.

M-4	$-\ln(C_t/C_0)$ vs. Time		
wraterial	Fitting Equations	R-Square	
MOF	Sigmoidal	$R^2 = 0.99947$	
BiOI	Linear	$R^2 = 0.9896$	
BiOI/MOF-30%	Linear	$R^2 = 0.99457$	
BiOI/MOF/F-BC-10%	Linear AND exponential	$R^2 = 0.99295$ $R^2 = 0.99342$	

Table S 2. Fitting parameters for the reaction course.



Figure S 5. Fitting of the reaction course for CIP degradation under simulated solar light catalyzed by pure BiOI. Markers are experimental point, line is the linear fitting (R^2 =0.9912).

Material	2 Theta (°)	Reflection (hkl)	d-spacing (Å)
BiOI	8.70	001	10.1
	29.09	102	3.06
	31.77	110	2.81
	45.45	200	1.99
	55.09	212	1.66
BiOI/MOF 30%	29.35	102	3.03
	31.91	110	2.80
	45.73	200	1.98
	55.35	212	1.66
BiOI/MOF 50%	30.07	102	2.96
	32.09	110	2.78
	45.97	200	1.97
	55.94	212	1.64
BiOI/MOF/F-BC 10%	28.98	102	3.07
	31.81	110	2.81
	45.60	200	1.98
	54.88	212	1.67
BiOI/MOF/F-BC 20%	28.98	102	3.07
	31.81	110	2.81
	45.60	200	1.98
	54.88	212	1.67

Table S 3. XRD analysis, reporting the observed angles of reflection of different crystalline planes and the calculated interplanar distances (Bragg law was used, so that the interplanar distance is $d = \frac{n\lambda}{2\sin\theta}$).



Figure S 6. XRD pattern of the oxidized biochar.

Figure S 7. UV spectrum along with the liquid chromatograms and mass-to-charge ratio spectra of the main photodegradation intermediates of ciprofloxacin generated in the photodegradation reaction catalyzed by the ternary composite (BiOI/MOF/F-BC 10%) at: (a) pH=3, (b) pH=6.2, (c) pH=9, and (d) pH=11.



a) pH=3































d) PH=11









