

Supporting Information

Comparison Between Different Mesoporous Carbons in the Removal of Doxycycline Antibiotic: Experimental Assays and Description of Adsorbate Features by Density Functional Theory (DFT)

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1. Characterization of prepared MPC

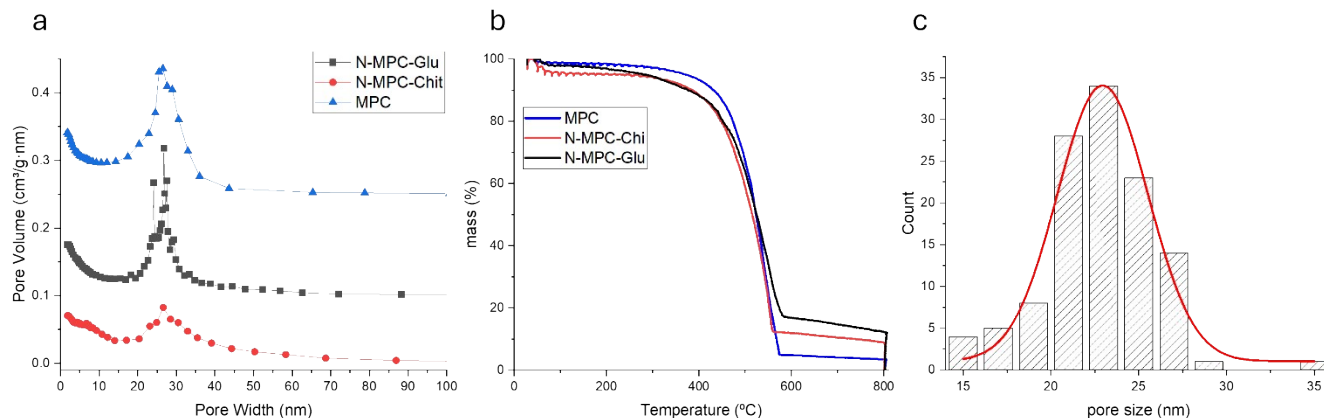


Figure S1 – (a) Pore size distribution of the carbonaceous materials, the distributions of N-MPC-Glu and MPC were offset by 0.1 and 0.25, respectively: (b)—TG analysis of carbonaceous materials, (c) pore size distribution of N-MPC-Chit derived from TEM analyses.

2. XPS analysis of prepared MPC

Table S1 – C-bond distributions from C1s XPS spectrum

Material	Csp ² (%)	Csp ³ (%)	C=O (%)	O-C=O (%)	O-C-O (%)	Carbonates (%)
MPC	53.2	30	9.5	4.6	2.7	-
N-MPC-Chi	58.5	22.1	8.7	5.0	3.7	2.0
N-MPC-Glu	68.7	19.7	6.3	5.3	-	-

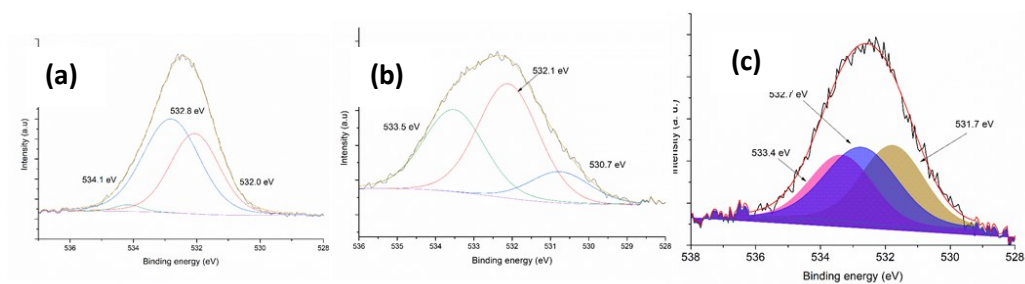


Figure S2 – O1s XPS spectrum of MPC (a); N-MPC-Chi (b); N-MPC-Glu (c).

Table S2 O-bond distributions from the O1s XPS spectrum

Material	Energy binding, percentage, functional group		
MPC	532.0 eV; 41.9%,	532.8 eV,	534.1 eV, 1.9%,
	COOH	56.2%, C-OH	C–O in anhydrides
N-MPC-Chi	531.7 eV, 28.2%,	532.7 eV,	533.4 eV 34.6%,
	COOH	37.2%, C-OH	C=O
N-MPC-Glu	530.7 eV, 13.4%,	532.1 eV,	533.5 eV,
	adsorbed H ₂ O	49.2%, COOH	37.4%, C=O

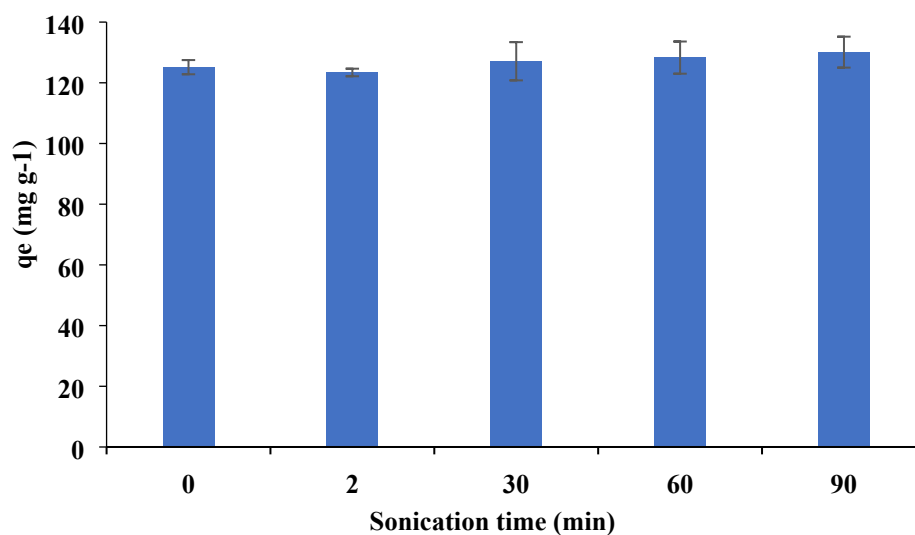


Figure S3– Influence of sonication assistance in the removal of DOX by N-MPC-Chi

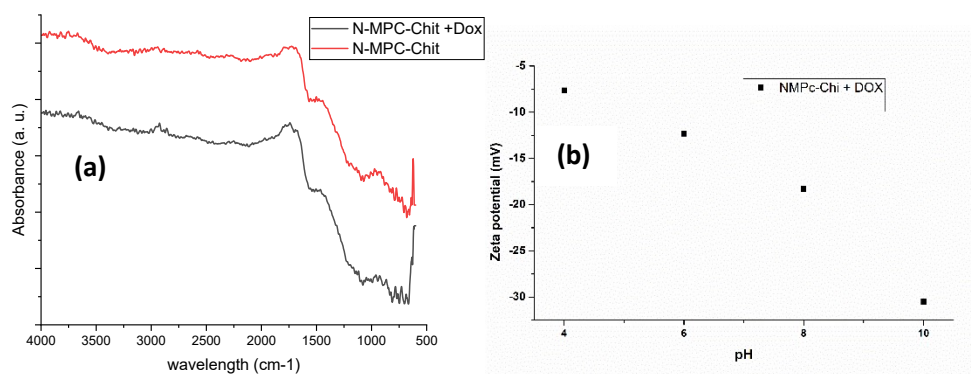


Figure S4 – (a) ATR-FTIR spectra of N-MPC-Chi and N-MPC-Chi/DOX loaded. (b) Zeta potential measurements of N-MPC-Chi + DOX.