Facile Synthesis of Mesoporous Carbon Nanocomposites from Natural Biomass for Efficient Dye Adsorption and Selective Heavy Metal Removal

Long Chen,¹ Tuo Ji,¹ Liwen Mu,¹ Yijun Shi,² Logan Brisbin,¹ Zhanhu Guo,³ Mohammel A. Khan,⁴ David P. Young⁴ and Jiahua Zhu^{1*}

¹Intelligent Composites Laboratory Department of Chemical and Biomolecular Engineering The University of Akron, Akron, OH 44325 USA

²Division of Machine Elements, Luleå University of Technology, Luleå, 97187, Sweden

³Department of Chemical and Biomolecular Engineering, University of Tennessee,

Knoxville, TN 37996, USA

⁴Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803,

USA

*Corresponding author: jzhu1@uakron.edu Phone: (330) 972-6859



Figure S1. TGA curve of C-00M.



Figure S2. BET isotherm of C-00M.



Figure S3. Change of (a) cumulative pore volume and (b) pore size distribution as a function of pore diameter of C-xxM.

The pore size distribution in the micropore region is calculated by density functional theory (DFT) method from CO₂ adsorption branch, and the one in the mesopore region is calculated by Barret Joyner and Halenda (BJH) method from N₂ adsorption branch. The combined pore size distribution is shown in Figure S3. Figure 3(a) shows the cumulative pore volume change as a function of pore diameter. Flattened curve was observed in C-00M with pore diameter larger than 2 nm. In C-xxM, a sharp increase of pore volume in 2<d<30 nm region clearly reveals the existence of mesopores. The pore size distribution is also interpreted in derivative pore volume against pore diameter, Figure 3(b). For C-00M, peaks were only found in micropore region, while peaks were detected in both micro- and meso-pore regions for C/Fe nanocomposites.



Figure S4. UV-Vis spectra with increasing MB concentration from 100 to 10000 ppb.



Figure S5. UV-Vis spectra with increasing MO concentration from 200 to 25000 ppb.

Non-linear fitting

The nonlinear mathematical form of the Langmuir model is expressed as:

$$q_e = \frac{k_1 q_{max} C_e}{1 + k_1 C_e}$$

Where c_e and q_e are dye concentration remained in the solution (mg/L) and the amount of dye adsorbed onto adsorbent (mg/g) at equilibrium, respectively. q_{max} is the maximum adsorption capacity (mg/g) and k_l represents the energy constant related to the energy of adsorption. q_e can be calculated by following Equation:

$$q_e = \frac{c_o - c_e}{m/V}$$

Where c_0 and c_e are initial and equilibrium pollutant concentrations (mg/L), *m* is the mass of adsorbent (g) and *V* is volume of polluted solution (L). Adsorption capacity q_{max} can be determined by fitting the data to Langmuir adsorption model using non-linear regression method. The nonlinear mathematical form of the pseudo-second-order kinetic model is expressed as:

$$q_t = \frac{{q_e}^2 k_2 t}{1 + q_e k_2 t}$$

Where *t* is the sampling time (min), q_t is the dye concentration on adsorbent at time *t* (mg/g), q_e is the amount of dye adsorbed on to adsorbent (mg/g) at equilibrium. k_2 is the pseudo-second-order rate constant (g/mg min).adsorption rate constant can be obtained by fitting the data to pseudo-second-order kinetic model.



Figure S6. Non-linear regression of MB adsorption data to Langmuir isotherm model (a) C-00M, (b) C-01M, (c) C-03M, (d) C-05M and (e) C-10M.



Figure S7. Non-linear regression of MO adsorption data to Langmuir isotherm model (a) C-00M, (b) C-01M, (c) C-03M, (d) C-05M and (e) C-10M.



Figure S8. Non-linear regression of MB adsorption data to pseudo-second-order kinetic model (a) C-00M, (b) C-01M, (c) C-03M, (d) C-05M and (e) C-10M.



Figure S9. Non-linear regression of MO adsorption data to pseudo-second-order kinetic model (a) C-00M, (b) C-01M, (c) C-03M, (d) C-05M and (e) C-10M.



Figure S10. Zeta potential of pure carbon and carbon nanocomposites.



Figure S11. [Fe] leached into aqueous solution during adsorption.

Sample	Adsorption Capacity (mg/g)	Surface Area (m²/g)	Adsorption Capacity (mg/m²)	Reference
С-03М	87.3	251.7	0.35	This work
				J. Hazard. Mater.,
AC-cotton stalk	193.5	794.8	0.24	2009, 166, 1514-
				1521
AC-rattan sawdust	294	1896	0.16	Dyes Pigments,
				2007, 75, 143–149
AC-Waste apricot	102	1060	0.10	J. Hazard. Mater., 2006, B135 232–241

 Table S1. Comparison of surface property and MB adsorption capacity.

Table S2. Freundlich isotherm parameters for heavy metal ions adsorption with C-03M.

Mataliana	Parameters		
Ivietal Ions	K_{f}	n	
Zn(II)	1.00	0.91	
Ni(II)	0.92	0.88	
Cu(II)	9.08	1.69	
Cr(VI)	12.5	1.31	
Pb(II)	10.5	1.56	