Selective Removal of Iron, Lead, and Copper Metal ions from Industrial Wastewater by a Novel Cross-linked Carbazole-Piperazine Polymer

Majed Al Anazi[1], Ismael abdulaziz[2], Othman Charles S. Al Hamouz*[1,3]

[1]Chemistry Department, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia.
[2]Interdisciplinary Research Center for membranes and water security, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia.
[3]Interdisciplinary Research Center for Hydrogen and Energy Storage, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia.
Corresponding Author E-mail: othmanc@kfupm.edu.sa; (Cell: +966552709130)

1. Molecular Simulation

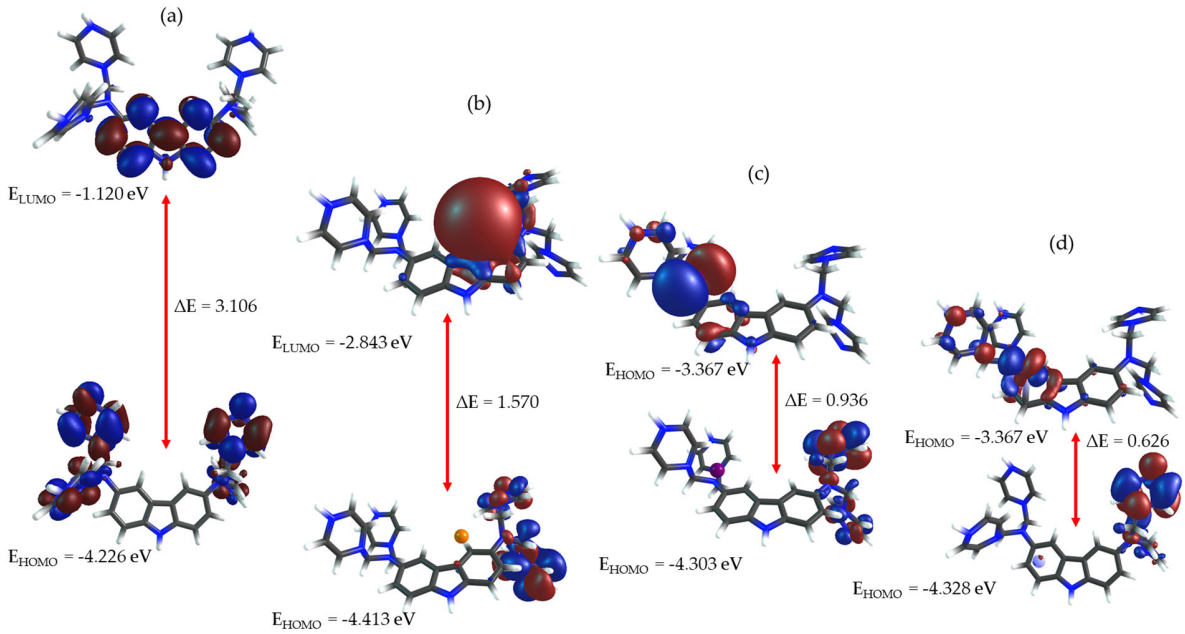

Figure S1. The change in frontier molecular orbital distribution of (a) ***MXM*** when interacting with (b) Cu^{2+}, (c) Pb^{2+} and (d) Fe^{2+} ions at the B3LYP/6-311G* & SDD levels of theory.

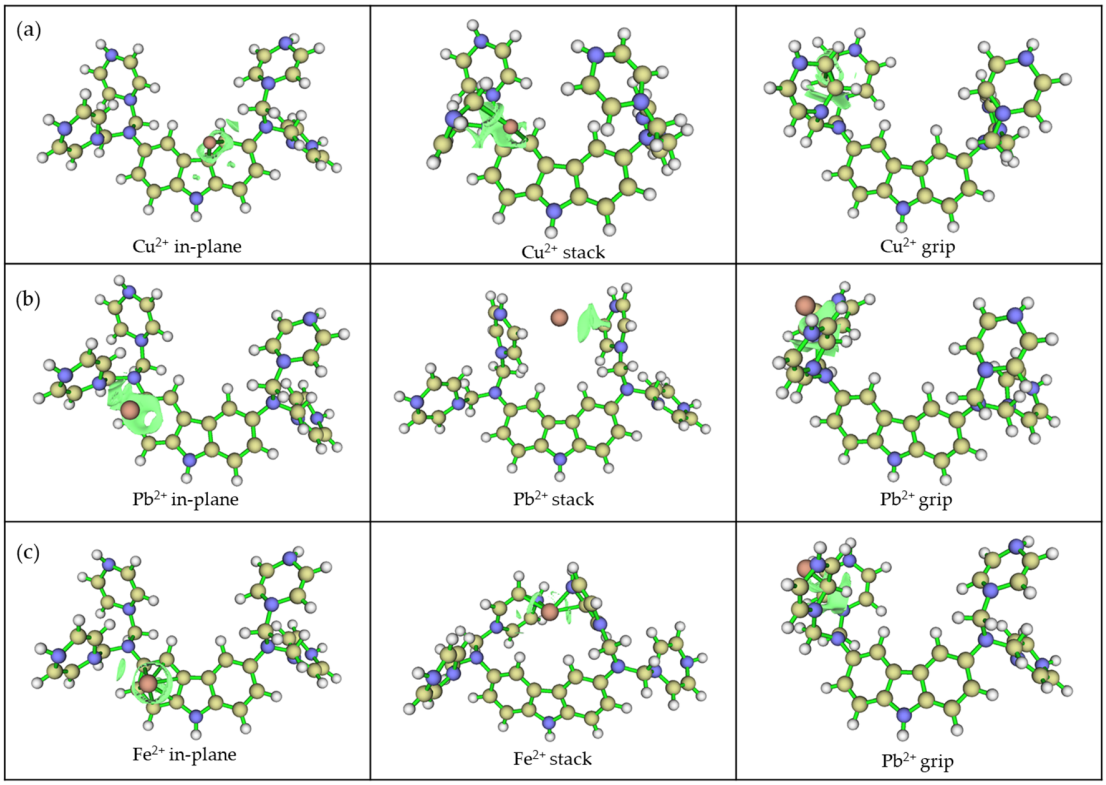

Figure S2. The reduced density gradient (RDG) isosurface plots of the interactions of ***MXM*** with (a) Cu^{2+}, (b) Pb^{2+} and (c) Fe^{2+} ions

2. Swelling properties

In a typical experiment; a 0.1 g of MXM polymer was weighed before the swelling experiment and was recordered as M_o. the sample was immersed in distill water for 24 hours. once the time was elapsed the sample surface was dried. The sample was weighed again (M_f) and the % swelling was measured as follow:

$$\%\ Swelling = \frac{M_f - M_o}{M_o} * 100 \qquad (1)$$

The results reveled that the % swelling was found 15 %.

3. Comparison table with literature:

Table S1. Comparison between ***MXM*** and adsorbents for the removal of heavy metal ions.

	% Removal			
Material	Fe	Pb	Cu	Reference
Carbon nanotube/G composite	-	-	83.3	[1]
Titanate nanotube/G nanocomposite	-	-	98	[2]
Chitosan	99.3	-	90	[3]
PE/PP non-woven fabric grafted with poly(bis[2-(methacryloyloxy) ethyl] phosphate)	-	-	60	[4]
γ-polyglutamic acid (γ-PGA) functionalized lignin (DLGS)	-	99.24	56	[5]
and ε-poly-L-lysine (ε-PL) functionalized lignin (DLLS)	-	99.04*	54*	[5]
poly (hydroxamic acid) ligand	99.3	-	90	[6]
phytic acid-functionalized spherical poly-phenylglycine	-	95	91	[7]
MXM	100*	96*	55*	This work

* Mixed metal ion solution

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