Transition Metal Doped MgO Nanoparticles for Nutrient Recycling: An Alternate Mg Source for Struvite Synthesis from Wastewater

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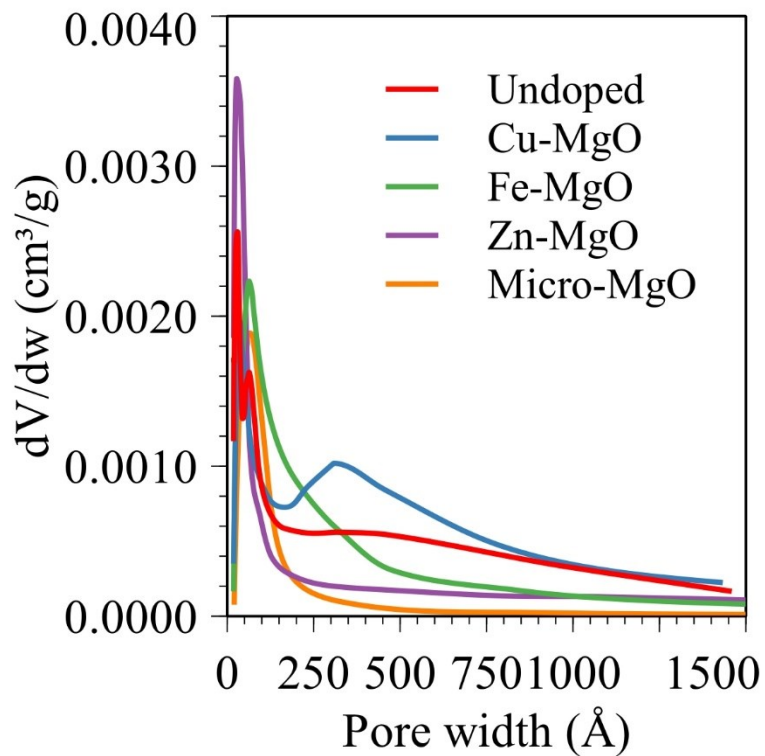*Corresponding author: job314@lehigh.edu, phone +1-610-758-6836

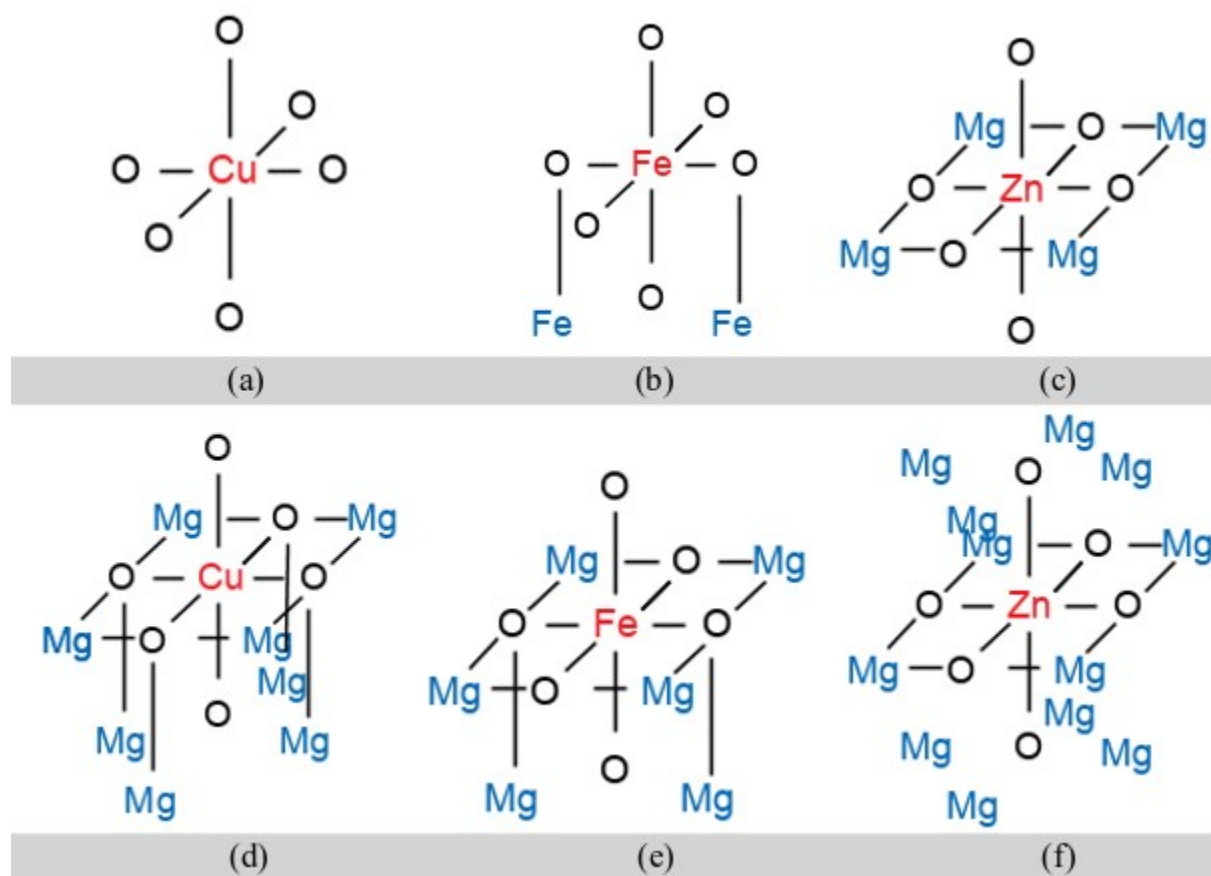Figure S1. Pore size distributions for MgO NPs and microcrystalline MgO.

Figure S2. Models used for EXAFS fitting

Table S1. Adsorption kinetic model fits for undoped and doped MgO with varying temperatures and time ranges.

Model	Sample Name	Time Range (min)	Temperature (°C)	Parameters		R^2
				q_e (mg g^{-1})	k_2 (g mg^{-1} min^{-1})	
Pseudo-second Order	Undoped	0-35	25	1666.67	9.00E-04	0.992
			35	1428.57	7.00E-04	0.998
			45	1428.57	7.00E-04	0.999
	Cu-MgO		25	1428.57	1.75E-04	0.973
			35	1428.57	2.33E-04	0.983
			45	1250.00	3.20E-04	0.989
	Fe-MgO		25	1666.67	2.43E-05	0.289
			35	3333.33	4.48E-06	0.046
			45	1666.67	1.90E-04	0.301
	Zn-MgO		25	1111.11	1.45E-04	0.894
			35	5000.00	1.06E-06	0.010
			45	1250.00	3.20E-04	0.989
Pseudo-second order	Undoped	0-5	25	1428.57	2.45E-03	0.971
			35	1250.00	2.13E-03	0.964
			45	1111.11	2.70E-03	0.971
	Cu-MgO		25	833.33	1.03E-03	0.806
	Fe-MgO			77.52	6.66E-02	0.102
	Zn-MgO			217.39	8.46E-03	0.246
				k_p	C	
Intraparticle diffusion	Undoped	0-5	25	618.25	31.928	0.988
	Cu-MgO			354.72	7.064	0.998
	Fe-MgO			134.40	30.435	0.815
	Zn-MgO			142.53	6.908	0.990
	Microcrystalline MgO			177.43	64.766	0.884

Table S2. Structural parameters (obtained from the fittings of K-edge EXAFS data) of the first two coordination shells around the dopant metal atom centers. The errors for R and σ^2 are within parentheses.

| Sample name	Bond	N	R(Å)	$\sigma^2(\text{Å}^2)$
Cu-MgO	Cu-O (eq.)	4	2.03 (.01)	.0080 (.0013)
	Cu-O (ax.)	2	2.31 (.03)	.0081 (.0035)
	Cu-Mg(Cu)	8	2.96 (.02)	.0095 (.0011)
Fe-MgO	Fe-O	6	1.95 (.0008)	.0113 (.0006)
	Fe-Mg(Fe)	6	2.98 (.011)	.0087 (.0007)
Zn-MgO	Zn-O	6	2.12 (.015)	.0075 (.0018)
	Zn-Mg(Zn)	12	3.00 (.015)	.0066 (.0011)
Cu-Struvite	Cu-O (eq.)	4	1.96 (.010)	.0058 (.0005)
	Cu-O (ax.)	2	2.3 (0.1)	.035 (.016)
Fe-Struvite	Fe-O	6	1.97 (.004)	.0093 (.0002)
	Fe-Mg(Fe)	2	3.05 (.007)	.0127 (.0009)
Zn-Struvite	Zn-O	6	1.98 (.024)	.0123 (.0014)
	Zn-Mg(Zn)	4	2.95 (.030)	.0101 (.0027)
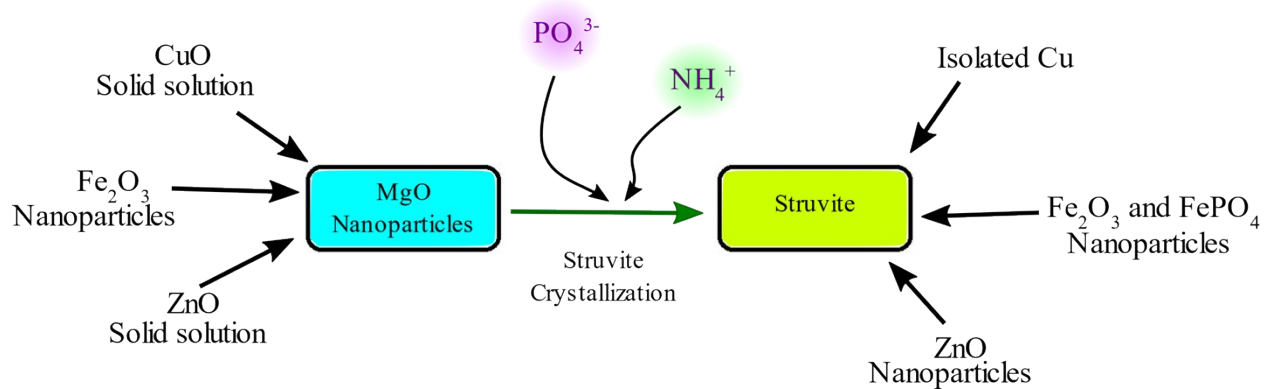
Figure S3. Summary of reaction process and fate of the dopants in MgO.