Cu(II) coordination polymer-based catalytic sensing system for detecting cysteine and sulfur anions

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Supporting Information



Fig.S1 EDS of Cu-Asp CP. The contents calculated for Cu-Asp CP were Cu of 33.93, C of 32.83, N of10.41, O of 22.83, respectively.



Fig. S2 The difference between the binding energies of before and after the binding reaction were 35.7949661 eV (a), 19.9081206 eV (b), 16.0552706 eV (c), respectively; the total binding energies of the systems were calculated to be - 64757.952eV (a), -76586.188eV (b), -135108.868eV (c), respectively.(a) Cu (Asp) (H₂O)₃, (b) Cu (Asp)₂(H₂O)₂, (c) Cu₂(Asp)₃(H₂O)₂.

B3LYP/6-31+G* level calculation was performed based on Gaussian 09, referred to the following,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.



Fig.S3 TG of Asp (red), Cu(NO₃)₂ (blue), Cu-Asp CP (black), respectively.



Fig.S4 N₂ sorption isotherm curve of Cu-Asp CP. The inset shows the corresponding pore size distribution. The specific surface area of the Cu-Asp CP was calculated from N₂ isotherm and was found to be 8.3 m²·g⁻¹. The corresponding pore size distribution reveals that Cu-Asp CP has small mesopores of *ca*.3.4 nm diameter, determined by using the BJH method.



Fig. S5 Comparison of the peroxidase-like activity of Cu^{2+} ions (red) and Cu-Asp CP (blue) towards the TMB-H₂O₂ system. [Cu²⁺ ions] = 69 μ M, [Cu-Asp CP] = 69 μ M, [TMB] = 0.5 mM, [H₂O₂] = 4 mM, 200 mM NaOAc–HOAc buffer solution of pH 4.0, temperature of 30 °C.