A ligand-chirality controlled supramolecular hydrogel

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Electronic Supplementary Information (ESI)

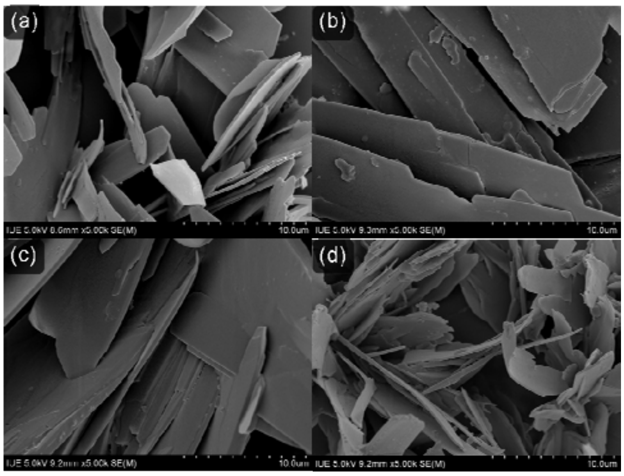


Figure S1 FESEM images of xerogels from the original metallogels containing *D*-Phe-Cu(II) of 0.35 % (a), 0.55 % (b), 0.7 % (c), and 1.4 % (d) by weight. Scale bar for (a-d) is 10 μm.

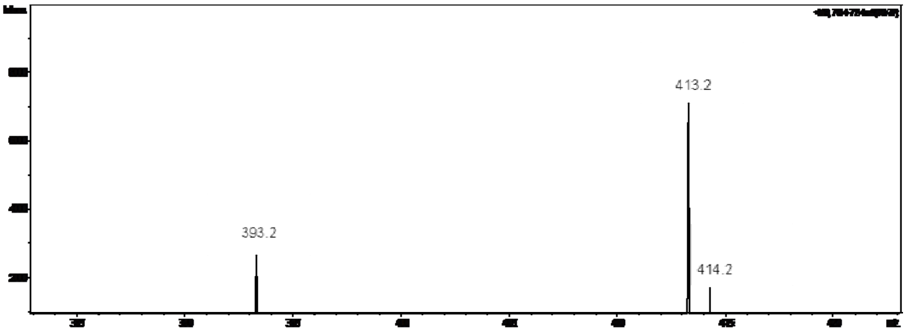


Figure S2 ESI-MS of the *L*-Phe-Cu(II) complex in acetonitrile/H_2O (1:1 by volume)

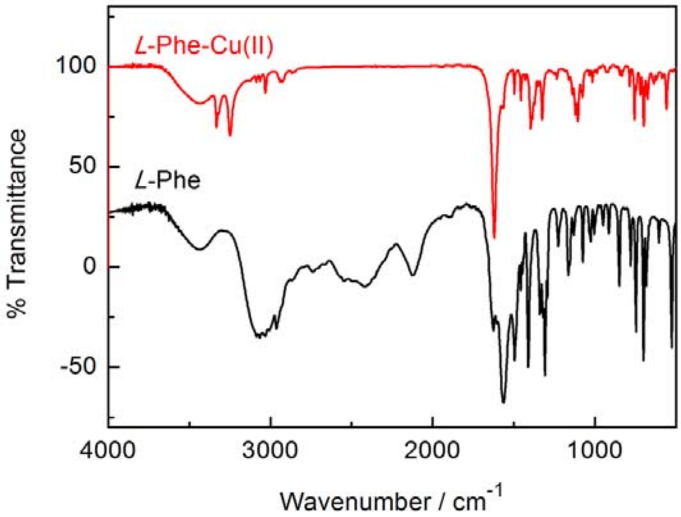


Figure S3 IR spectra of *L*-Phe (black) and *L*-Phe-Cu(II) xerogels from the original metallogel containing *L*-Phe-Cu(II) of 0.7 % by weight (red) in KBr pellets

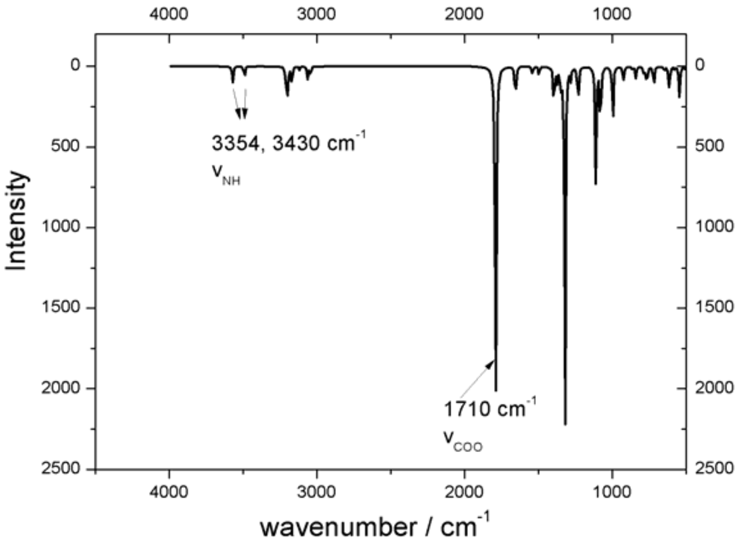
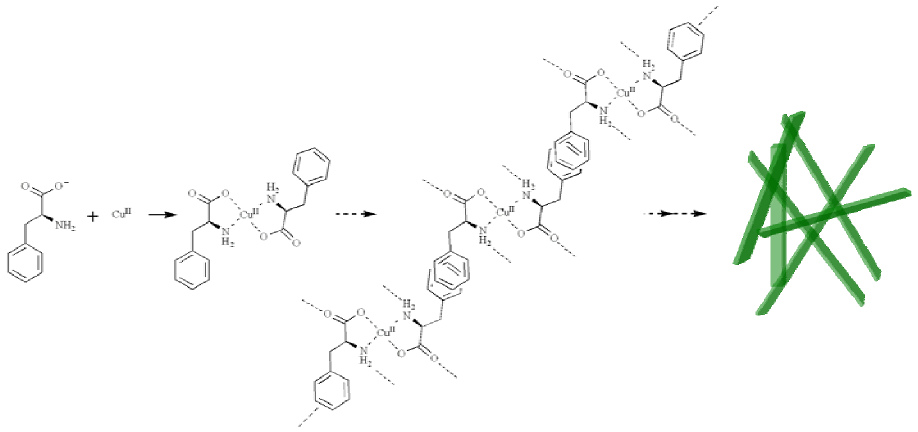


Figure S4 Gas-phase molecular mechanics simulative IR spectra of Phe-Cu(II) at B3LYP/6-31G9* level[1]

DFT calculation was performed based on Gaussian 03, referred to the following,

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M.

Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian 03, Revision A.1, Gaussian, Inc., Pittsburgh PA, 2003.



Scheme S1 Self-assembled superstructure model of the supramolecular metallogel of Phe-Cu(II)

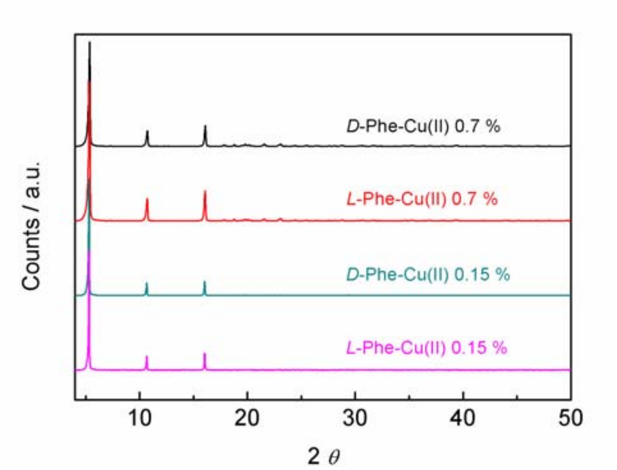
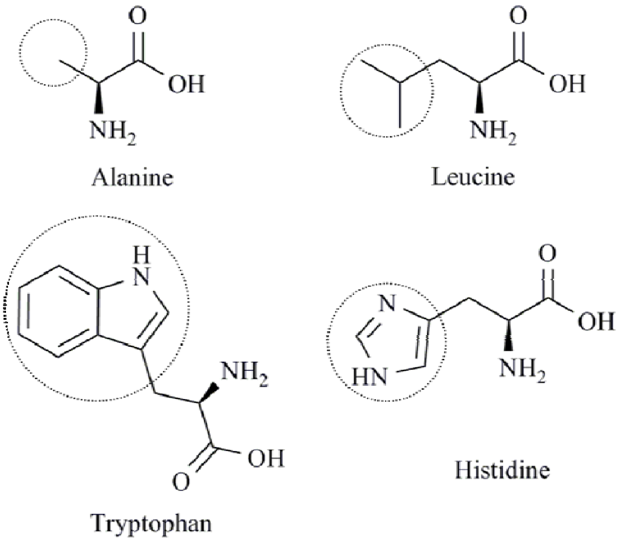


Figure S5 X-ray diffraction patterns of *D*-Phe-Cu(II) 0.7 %, *L*-Phe-Cu(II) 0.7 %, *D*-Phe-Cu(II) 0.15 %, and *L*-Phe-Cu(II) 0.15 % by weight.



Scheme S2 Molecular structures of the tested amino acid ligands

Table S1 Ionic strength effect on the formation of Phe-Cu(II) metallogel

[NaCl] / mM	Gelation, Y/N[a]
10	Y
50	Y
100	Y
300	Y
500	Y

[a]. The employed solution contained 0.7 % *L*-Phe-Cu(II) (wt). "Y/N" represents "Yes or No".

Table S2 Supramolecular hydrogels formation was examined by other metal ions than Cu(II)

M^{n+}	Gelation, Y/N[a]
Fe^{2+}	N
Co^{2+}	N
Fe^{3+}	N
Zn^{2+}	N
Cd^{2+}	N
Pb^{2+}	N
Ag^{+}	N

[a] The employed solution contained 0.7 % *L*-Phe-M^{n+} (wt). "Y/N" represents "Yes or No".