# Supporting Materials

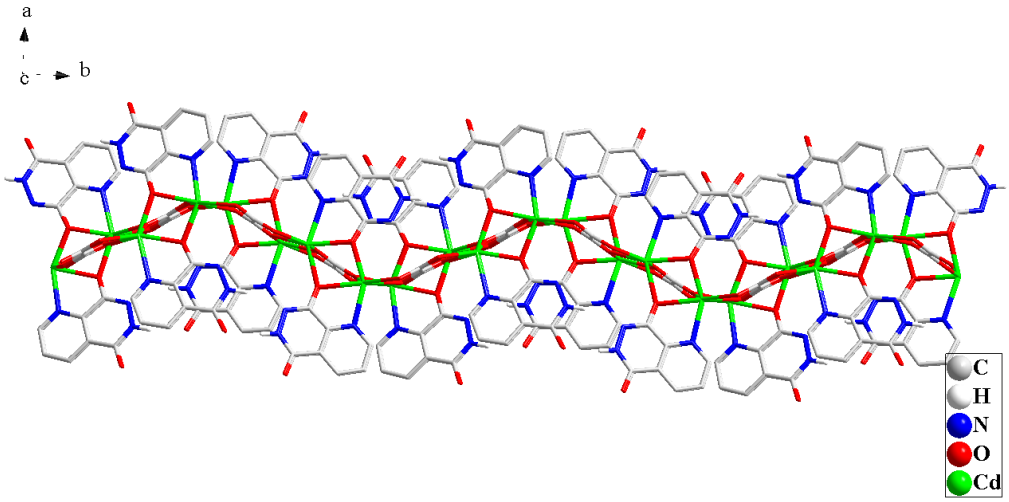
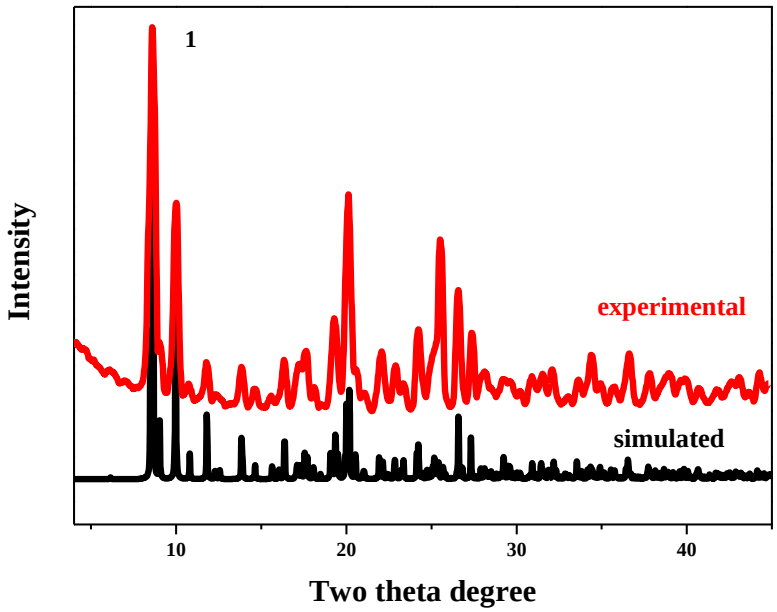



**Fig. S1** The projection plot of 2-D layer for compound **2** in *ab* plane.



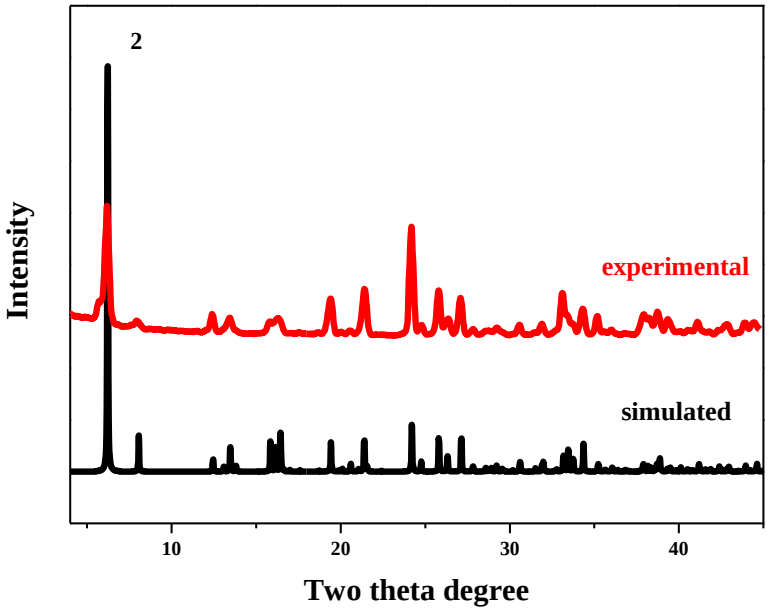
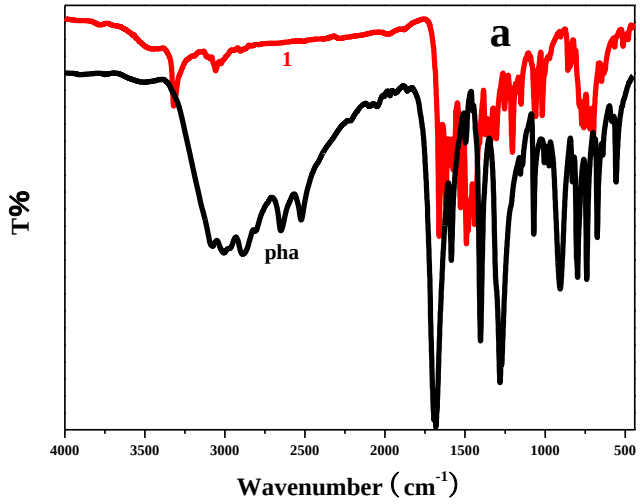



**Fig. S2** The simulated (black) and experimental (red) powder XRD patterns for compounds **1** and **2**.



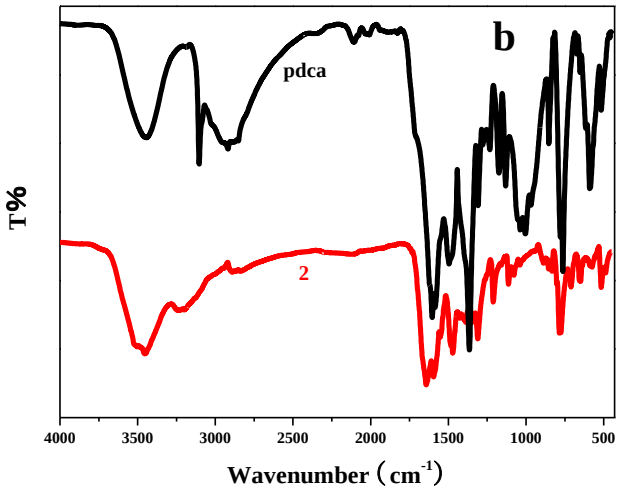



**Fig. S3** The IR spectrum of compounds **1** and **2**.

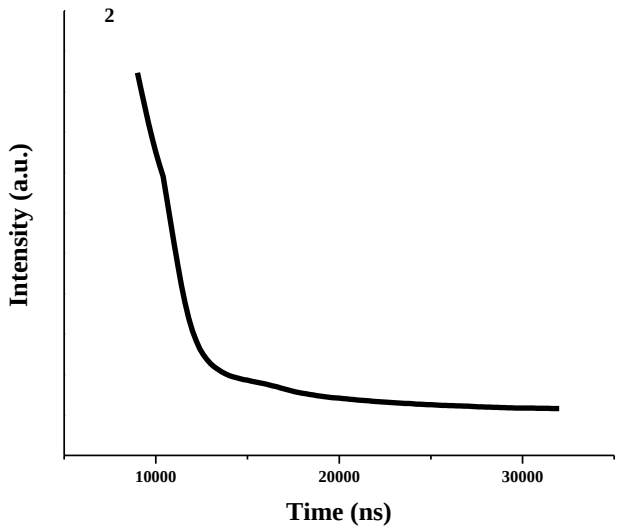
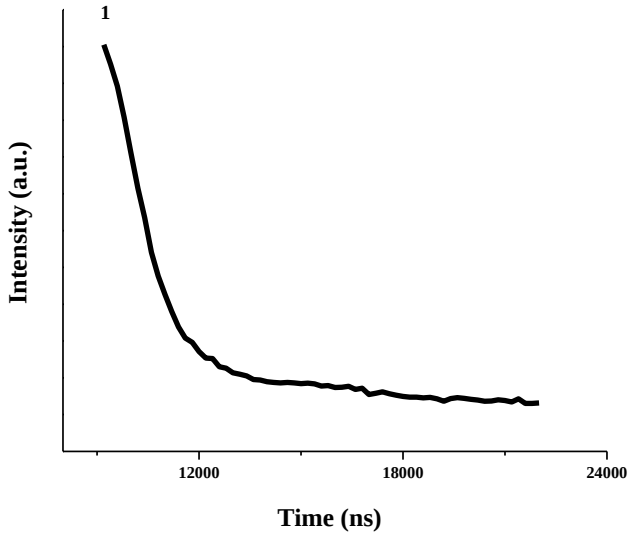



**Fig. S4** The experimental decay curve for the solid state compound **2**.



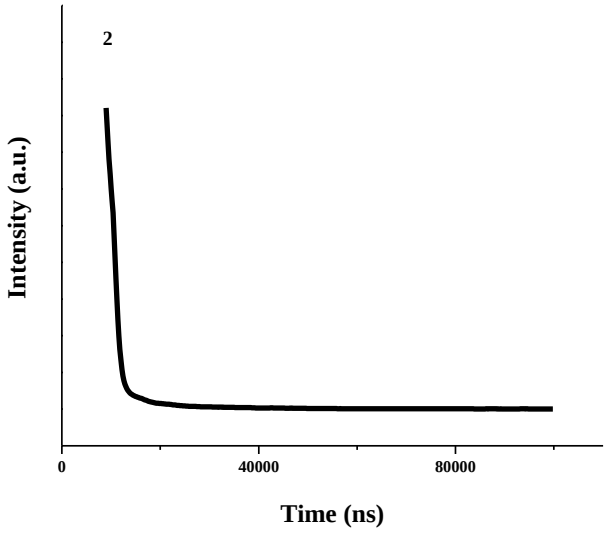
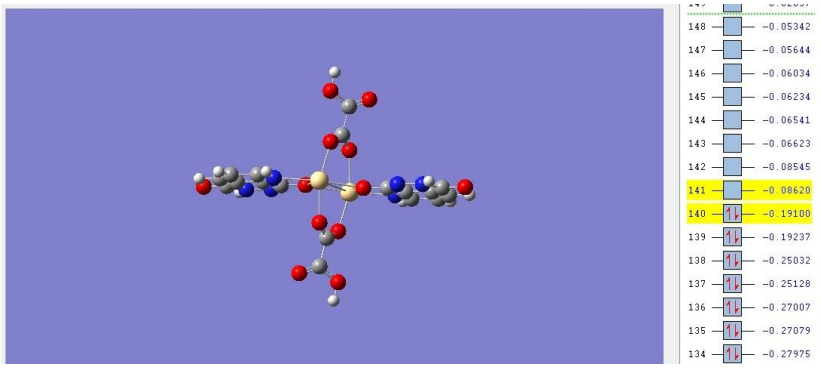




**Fig. S5** The experimental decay curves for compounds **1** (above) and **2** (bottom) in an aqueous solution.




(a)

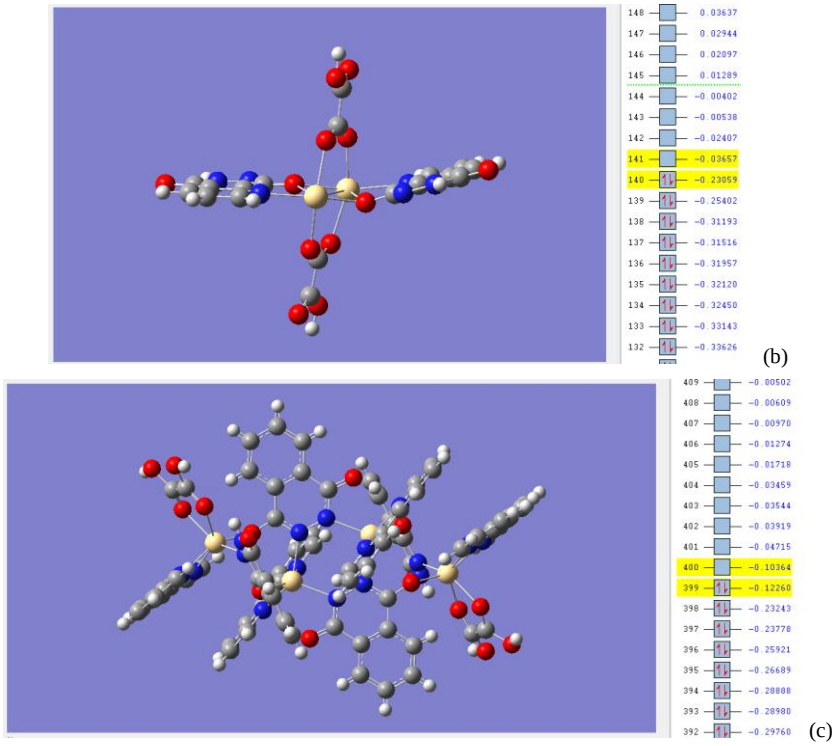



**Fig. S6.** The first singlet excited state structures for the solid-state compound **2** (a), compounds **2** (b) and **1** (c) in an aqueous solution.

Computational details for DFT calculations

The optimized geometric structure for the excited states of the solid-state compound **2** was performed with the TD-LC-wPBE method.[1] The calculations for non Cd atoms was carried out with 6-31g(d) basis set,[2] while for Cd atom with LanLDZ basis set.[3] The emission spectra was obtained using the time-dependent density functional theory TD-B3LYP.[4] All calculations were performed with the GAUSSIAN 09 program package.[5] The molecular orbitals were plotted with the GaussView program.[6]

**References**

1 (*a*) Y. Tawada, T. Tsuneda, S. Yanagisawa, T. Yanai, and K. Hirao, *J. Chem. Phys.*, 2004, **120**, 8425; (*b*) O. A. Vydrov and G. E. Scuseria, *J. Chem. Phys.*, 2006, **125**, 234109; (*c*) F. Furche and R. Ahlrichs, *J. Chem. Phys.*, 2002, **117,** 7433.

2 M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, D. J. DeFrees, J. A. Pople, and M. S. Gordon, *J. Chem. Phys.*, 1982, **77**, 3654.

3 P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.

4 (*a*) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (*b*) R. Bauernschmitt and R. Ahlrichs, *Chem. Phys. Lett.*, 1996, **256**, 454.

5 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 09 Revision B.02, Gaussian, Inc., Wallingford CT, 2010.

6 R. II. Dennington, K. Todd, J. Millam, K. Eppinnett, W. L. Hovell and R. Gilliland, GaussView, version 5.08, Semichem, Inc Shawnee Mission, KS, 2003.

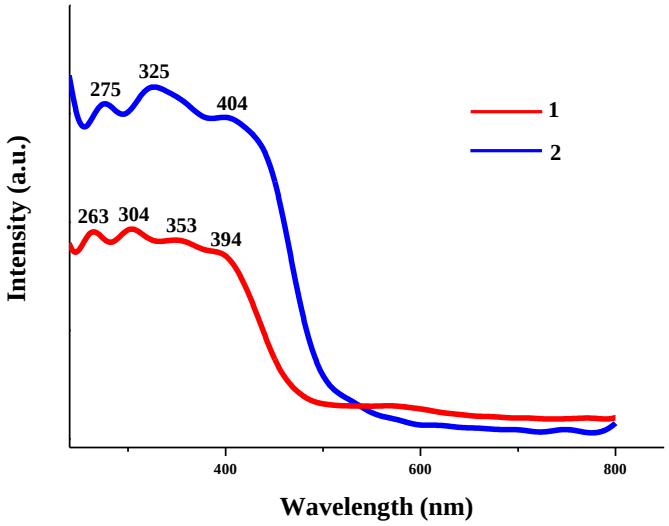



**Fig. S7** The electronic absorption spectra of compounds **1** and **2** in the solid state.

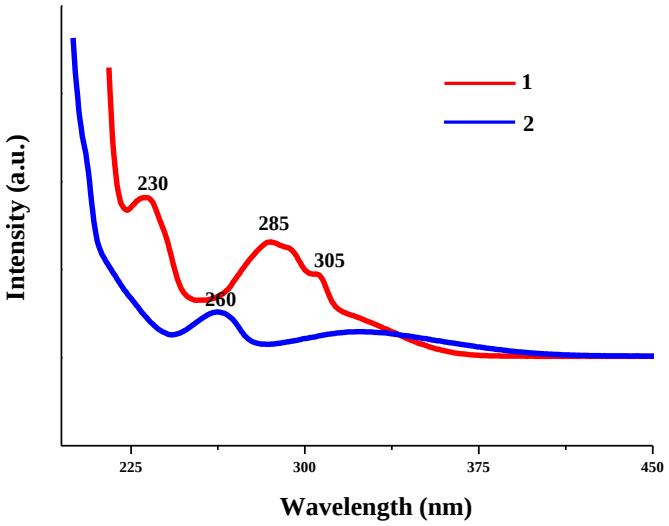



**Fig. S8** The electronic absorption spectra of compounds **1** and **2** in an aqueous solution.