**Calculation details:**

Electronic structure calculation was based on density function theory (DFT),\(^1\) in which wave functions were explained in a plane wave basis set and the spin polarized version of the PW-91 GGA was employed for the exchange-correlation functional in the CASTEP code.\(^2\)


Fig. S1  Packing diagram of 1
Fig. S2  PDOS of compound 1
Fig. S3 PDOS of compound 2