Supplementary information to

Effect of spin-phonon interaction on Urbach tails in flexible [$M_2(bdc)_2(dabco)$]

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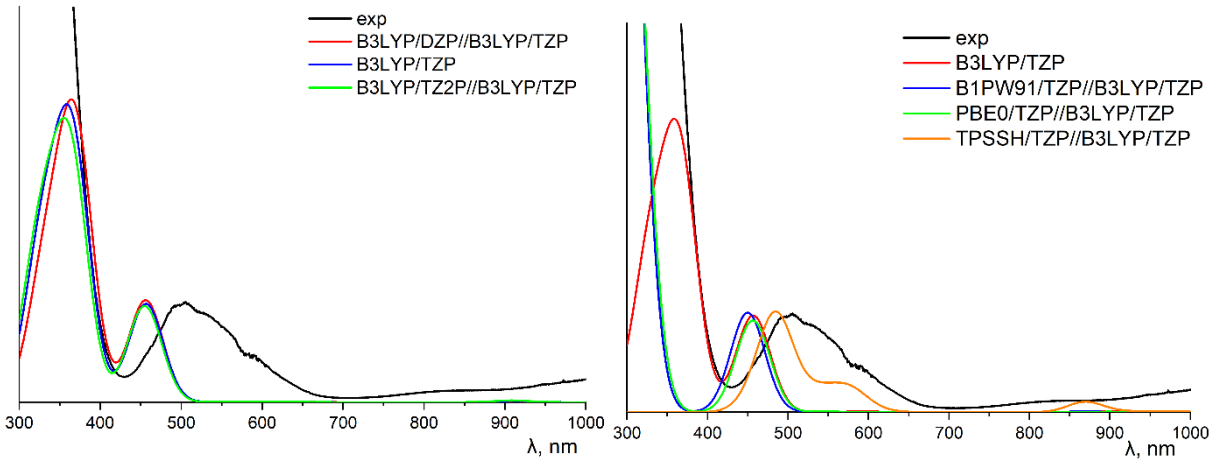

Fig. S1. Stability of the calculated absorption spectra relative to the basis set size (left) and density functional choice (right) for Co-DMOF. The absorption spectra calculated by B3LYP functional provide best reproduction of Kubelka—Munk functions in the region of intense absorption (300-400 nm).

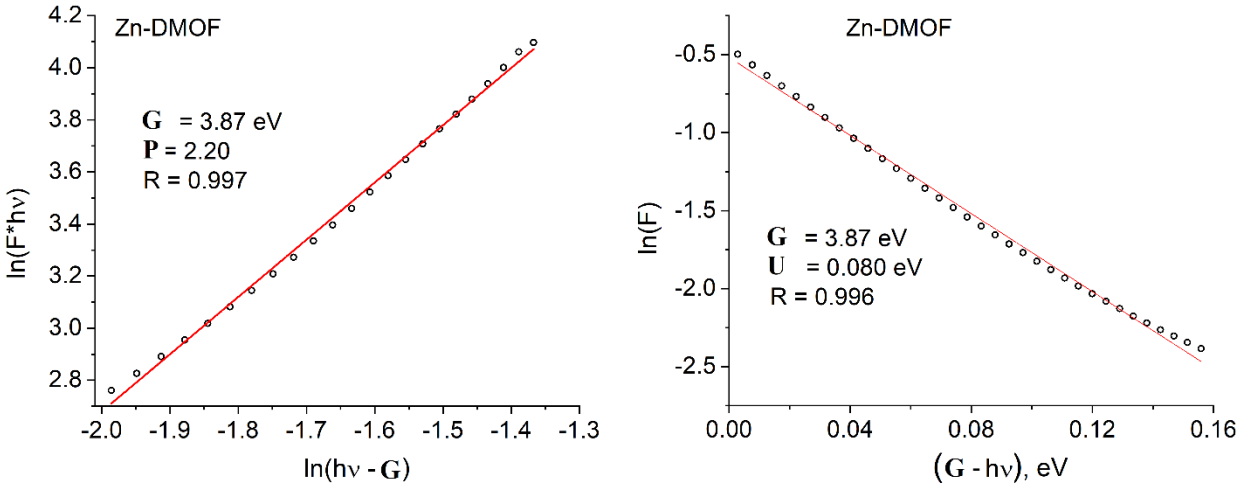

Fig. S2. Determining exponents P and **U** for Zn-DMOF.

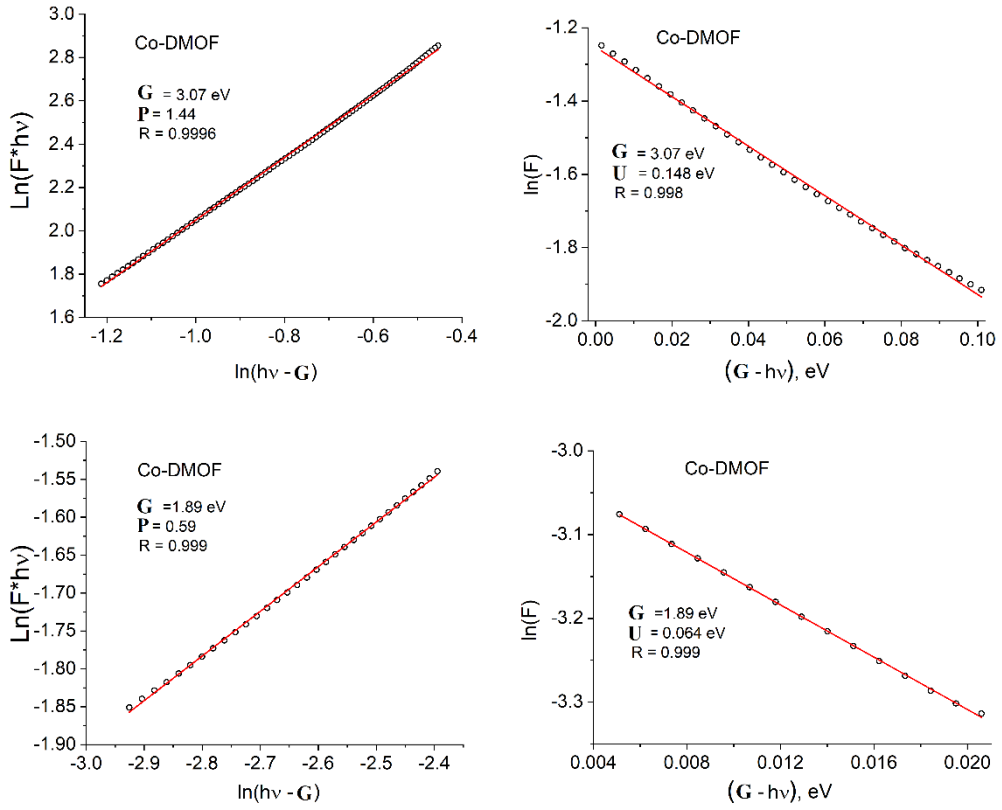

Fig. S3. Determining exponents P and **U** for Co-DMOF.

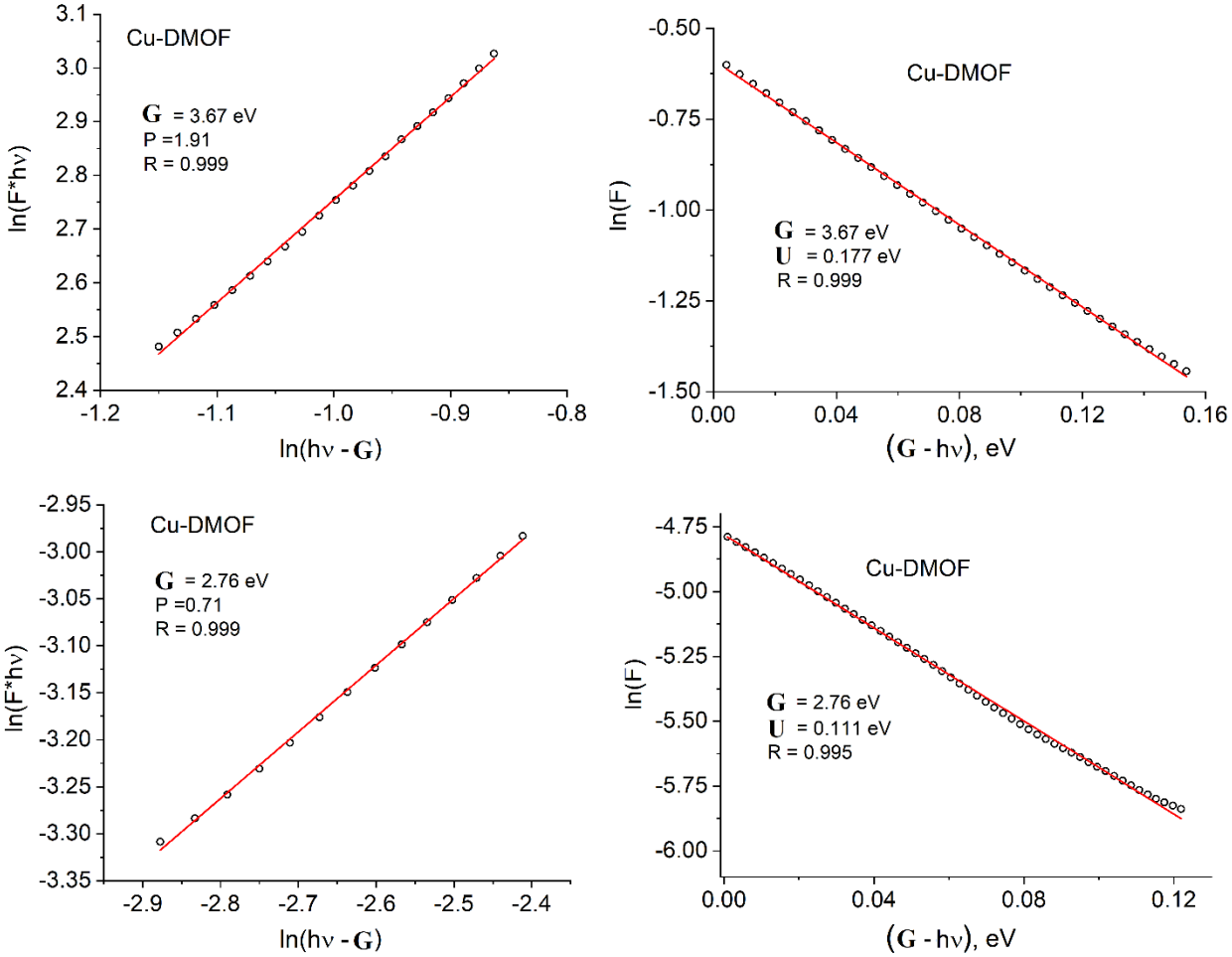

Fig. S4. Determining exponents P and **U** for Cu-DMOF.

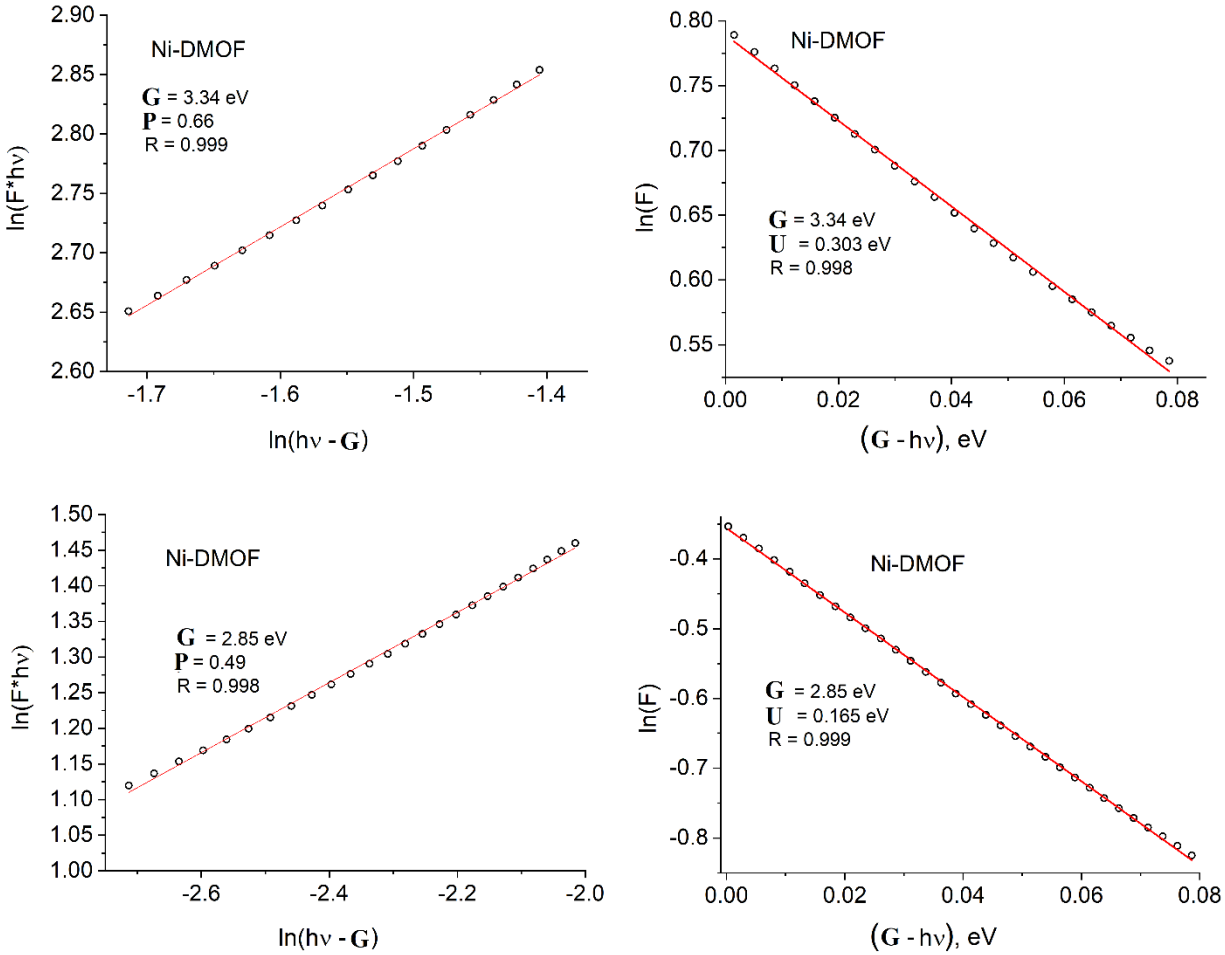

Fig. S5_1. Determining exponents P and **U** for Ni-DMOF.

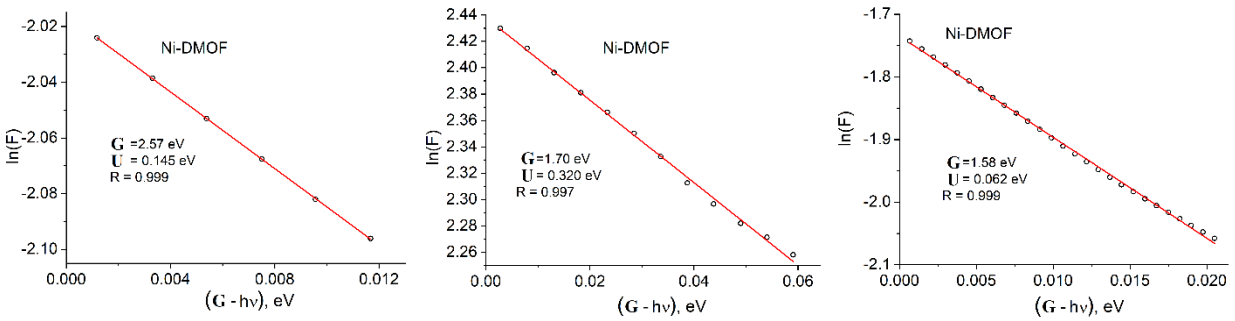

Fig. S5_2. Determining **U** for Ni-DMOF.

Table S1. Optimized geometry parameters for the $M_2(O_2CH)_4$ paddle-wheel model system.

	M-M, Å	M-O, Å	O-C, Å	<M-M-O, °	<O-M-M-O, °
$Zn_2(O_2CH)_4$	2.650	2.028	1.262	84.6	0.0
$Cu_2(O_2CH)_4$	2.506	1.965	1.263	86.6	0.0
$Ni_2(O_2CH)_4$	2.674	1.982	1.262	84.1	0.0
$Co_2(O_2CH)_4$	2.583	2.006	1.263	85.4	0.0

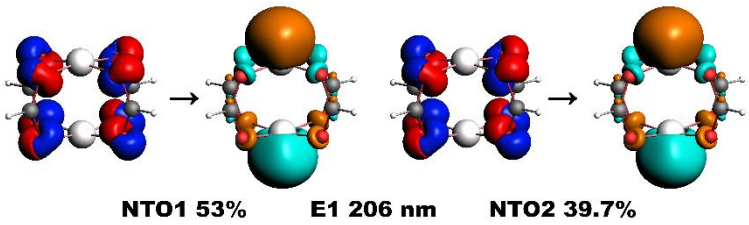

Fig. S6. NTOs for the most intense transition in $Zn_2(O_2CH)_4$

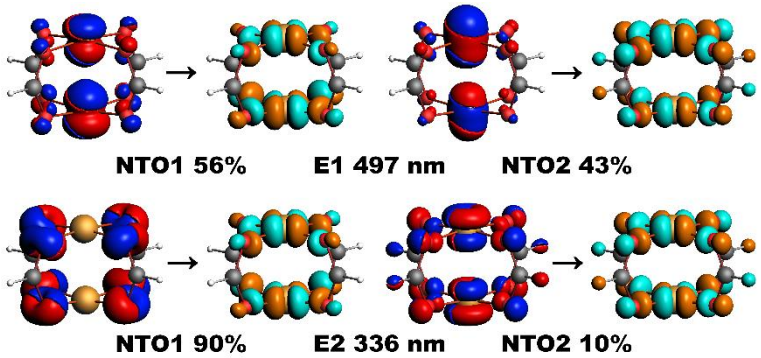

Fig. S7. NTOs for some most intense transitions in $Cu_2(O_2CH)_4$

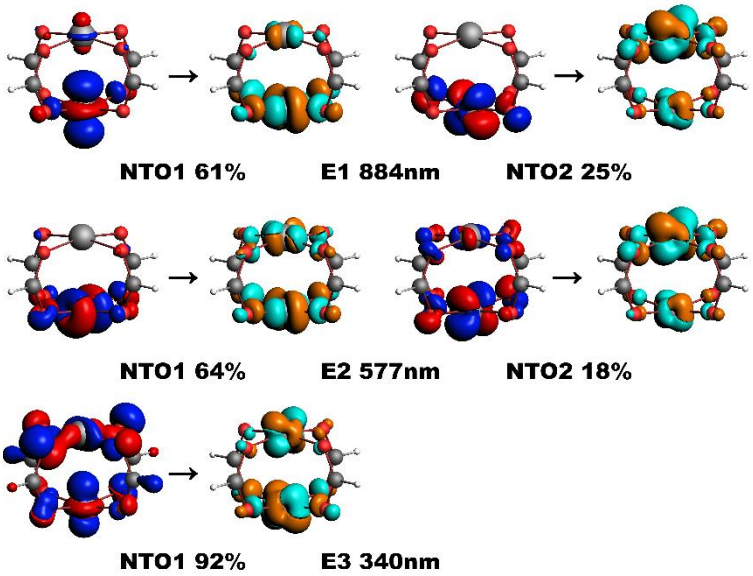

Fig. S8. NTOs for some most intense transitions in $Ni_2(O_2CH)_4$

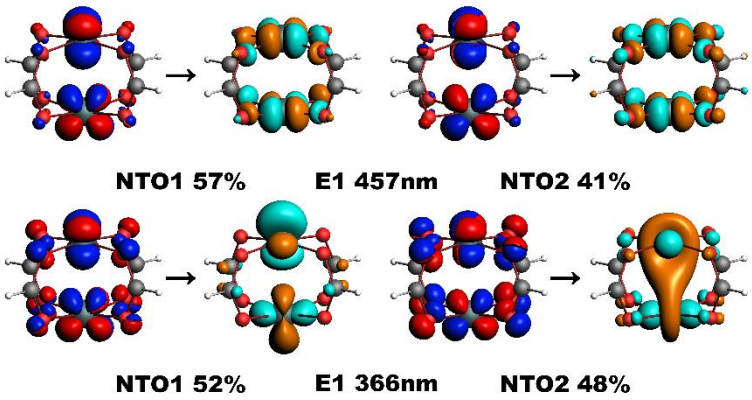

Fig. S9. NTOs for some most intense transitions in $Co_2(O_2CH)_4$