

Supporting Information for

Impact of diffusion methods and metal cations on photochromic three-component D-A hybrid heterostructures

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1. Crystal data and structure refinement parameters

Table S1. Crystal data and structure refinement parameters for the crystals of **1-A**, **2-A**, **1-B** and **2-B**

Complexes	1-A	1-B	2-A	2-B
Empirical formula	C ₄₈ H ₂₄ Mo ₁₂ N ₈ O ₅₂ SiZn ₄	C ₄₈ H ₂₄ Mo ₁₂ N ₈ O ₅₂ SiZn ₄	C ₄₈ H ₃₂ Cd ₂ Mo ₁₂ N ₈ O ₅₂ Si	C ₄₈ H ₃₂ Cd ₂ Mo ₁₂ N ₈ O ₅₂ Si
Formula weight	2985.60	2985.60	2956.98	2956.98
Temperature/K	293(2)	293(2)	293(2)	293(2)
Crystal system	monoclinic	tetragonal	tetragonal	tetragonal
Space group	<i>I</i> 2/ <i>a</i>	<i>P</i> -4 <i>m</i> 2	<i>I</i> 4 ₁ / <i>amd</i>	<i>P</i> 4 ₁ 2 ₁ 2
<i>a</i> /Å	24.4203(5)	19.5638(6)	19.8634(12)	19.8472(11)
<i>b</i> /Å	27.6230(4)	19.5638(6)	19.8634(12)	19.8472(11)
<i>c</i> /Å	24.4269(6)	39.891(3)	39.282(9)	39.686(3)
α /°	90	90	90	90
β /°	111.175(2)	90	90	90
γ /°	90	90	90	90
Volume/Å ³	15364.9(6)	15268.1(13)	15499(4)	15633(2)
Z	4	4	4	4
ρ_{calc} /cm ³	1.291	1.668	1.267	2.908
μ /mm ⁻¹	5.918	3.992	1.267	3.718
F(000)	5688.0	7128.0	5624.0	13065.0
Reflections collected	12931	77361	4594	72116
Independent reflections	12931	18089	4594	18299
Data/restraints/parameters	12931/0/554	18089/0/314	4594/1/153	18299/0/355
Goodness-of-fit on F ²	0.963	2.411	0.946	1.295
R_1^a, wR_2^b (<i>I</i> > 2 σ (<i>I</i>))	$R_1 = 0.0701,$ $wR_2 = 0.2367$	$R_1 = 0.2648,$ $wR_2 = 0.5325$	$R_1 = 0.0960,$ $wR_2 = 0.2384$	$R_1 = 0.2524,$ $wR_2 = 0.5301$
R_1^a, wR_2^b (all data)	$R_1 = 0.0885,$ $wR_2 = 0.2514$	$R_1 = 0.4733,$ $wR_2 = 0.6012$	$R_1 = 0.1451,$ $wR_2 = 0.2671$	$R_1 = 0.4835,$ $wR_2 = 0.6224$

$$^a R_1 = \sum ||F_0| - |F_c|| / \sum |F_0|. \quad ^b wR_2 = \{ \sum [w(F_0^2 - F_c^2)^2] / \sum [w(F_0^2)^2] \}^{1/2}.$$

2. Infrared spectral analysis

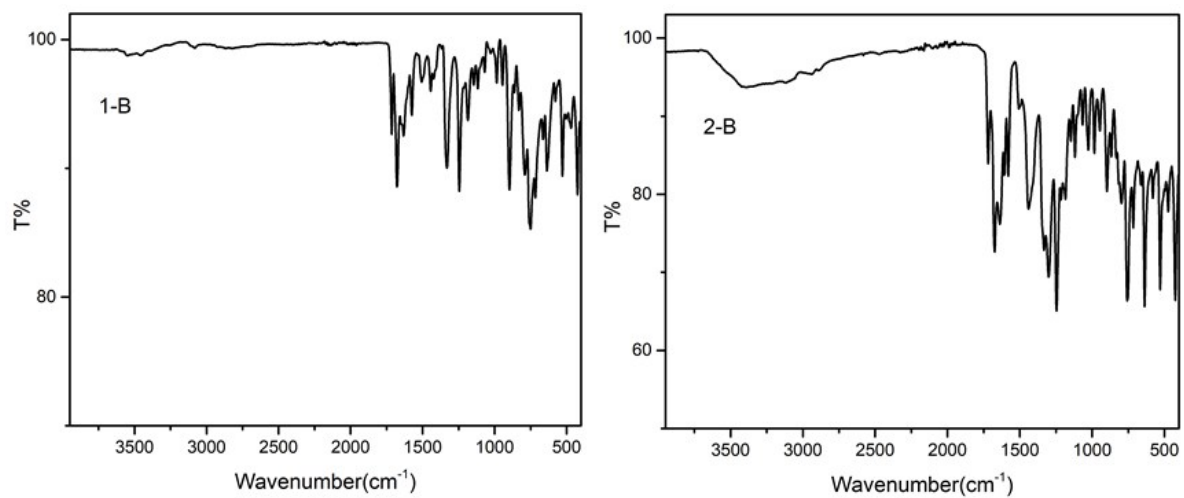


Fig. S1. Infrared spectra of hybrid complexes **1-B** and **2-B**

3. X-ray powder diffraction analysis

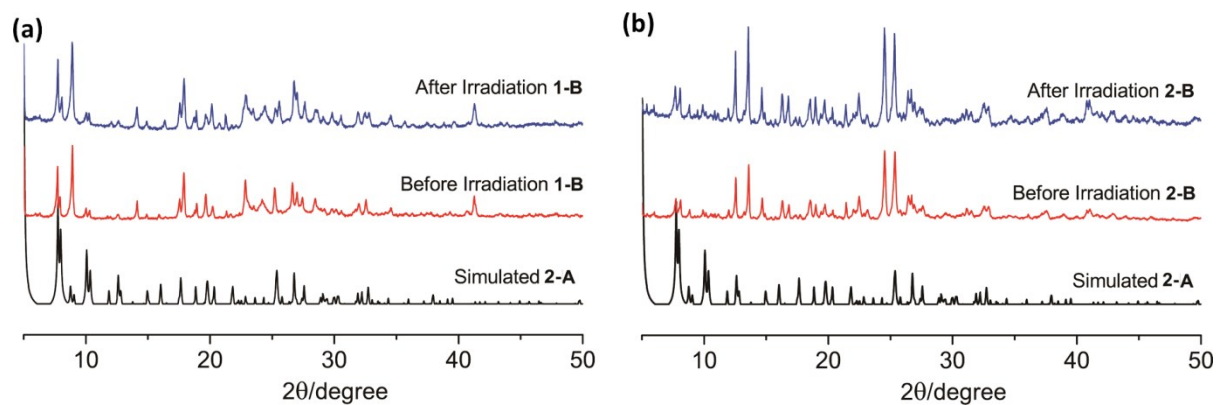


Fig. S2. The observed PXRD patterns for hybrid complexes **1-B**, **2-B** before and after irradiations, as well as that of the simulated **2-A**.