Electronic Supplementary Information (ESI)

for

Understanding the Vapochromic Response of Mixed Copper(I) Iodide/Silver(I) Iodide Nanoparticles toward Dimethyl Sulfide

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Figure S1. PXRD overlay of nanoparticle samples **1-3**.

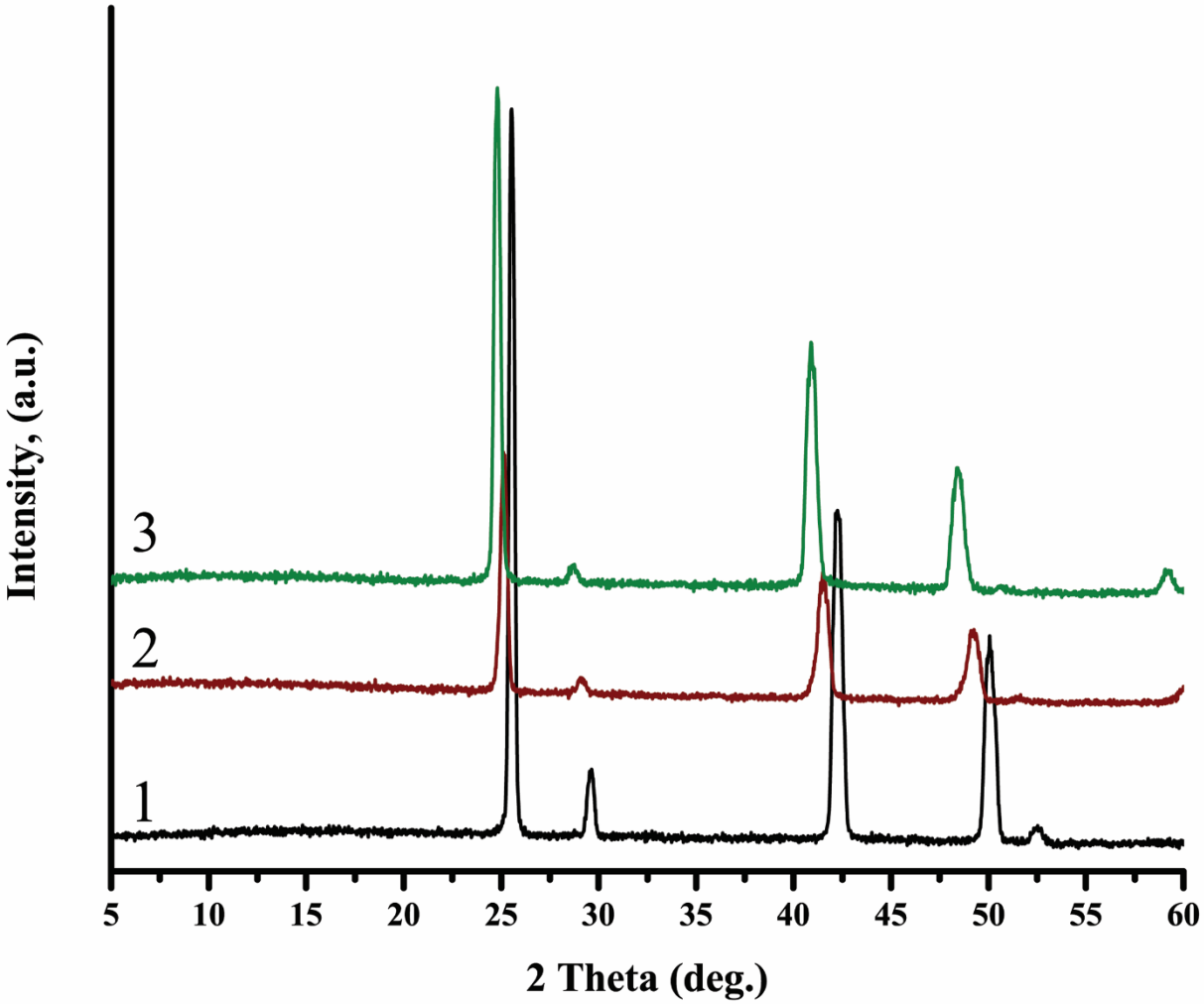

Figure S2. TEM micrograph images of nanoparticle samples **1-3**.

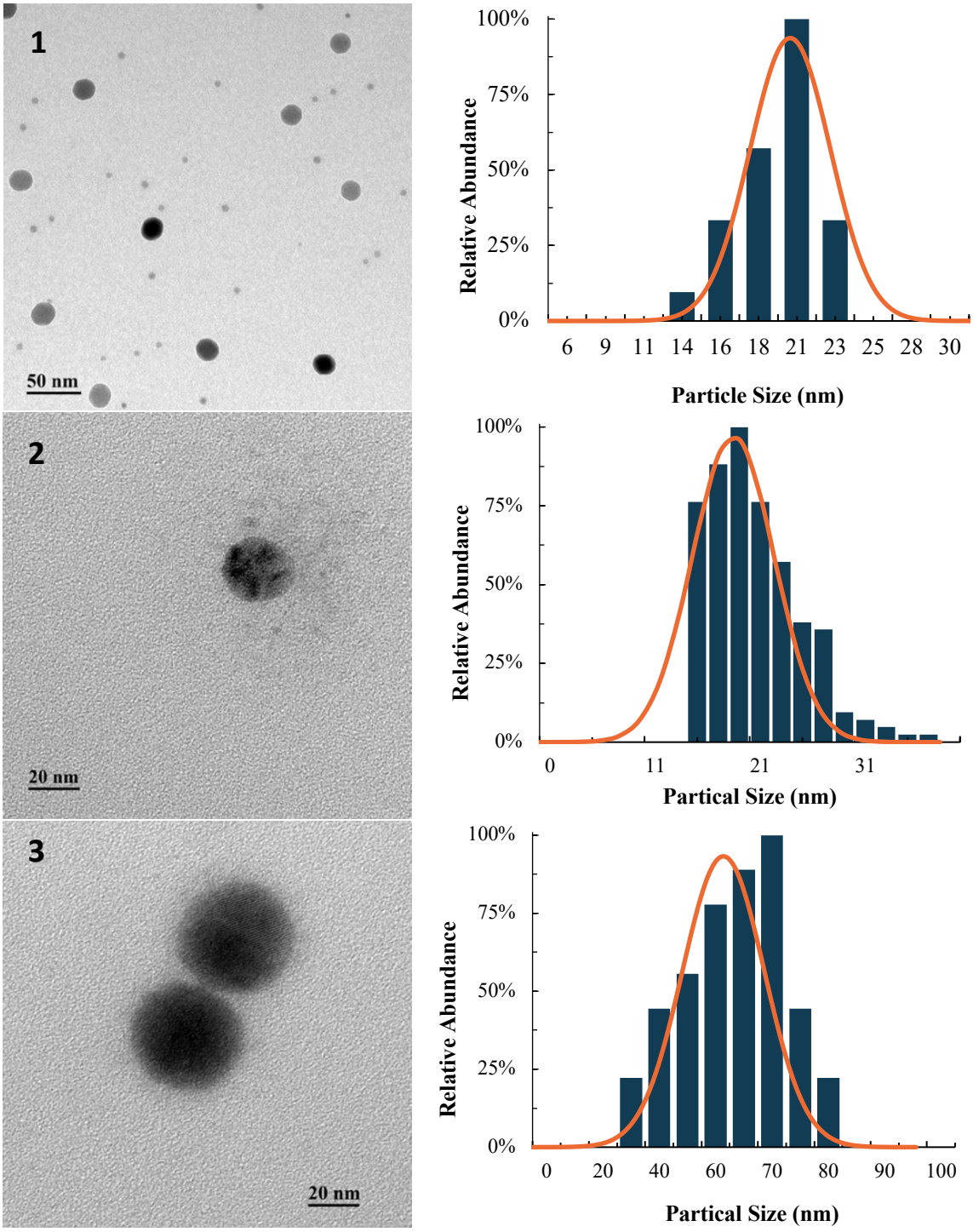

Figure S3. DRS spectra of solid samples of **1-3** at room temperature.

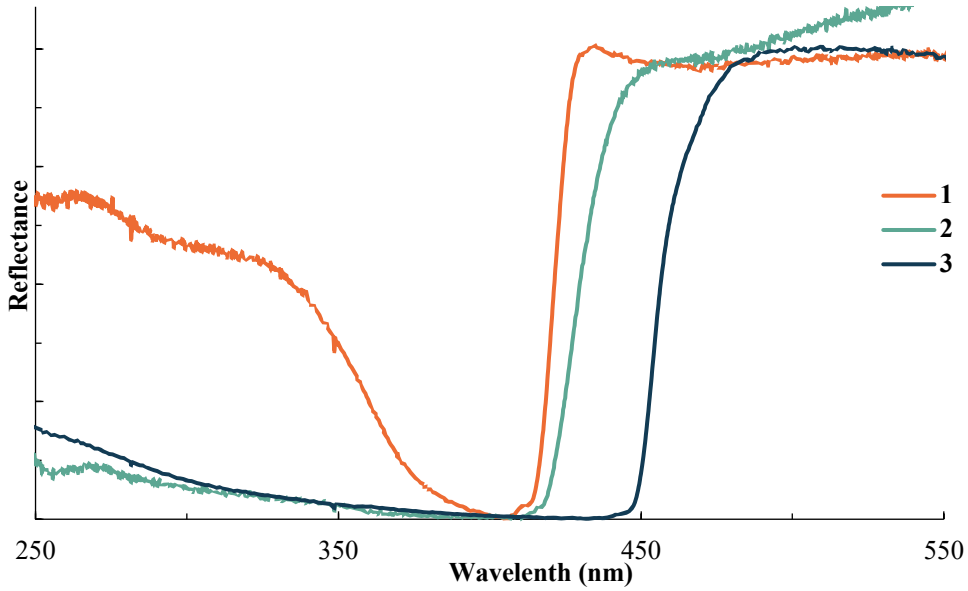

Figure S4. TGA comparisons of **1′-3′** before and after vacuum treatment (3 days, 100 μm vacuum).

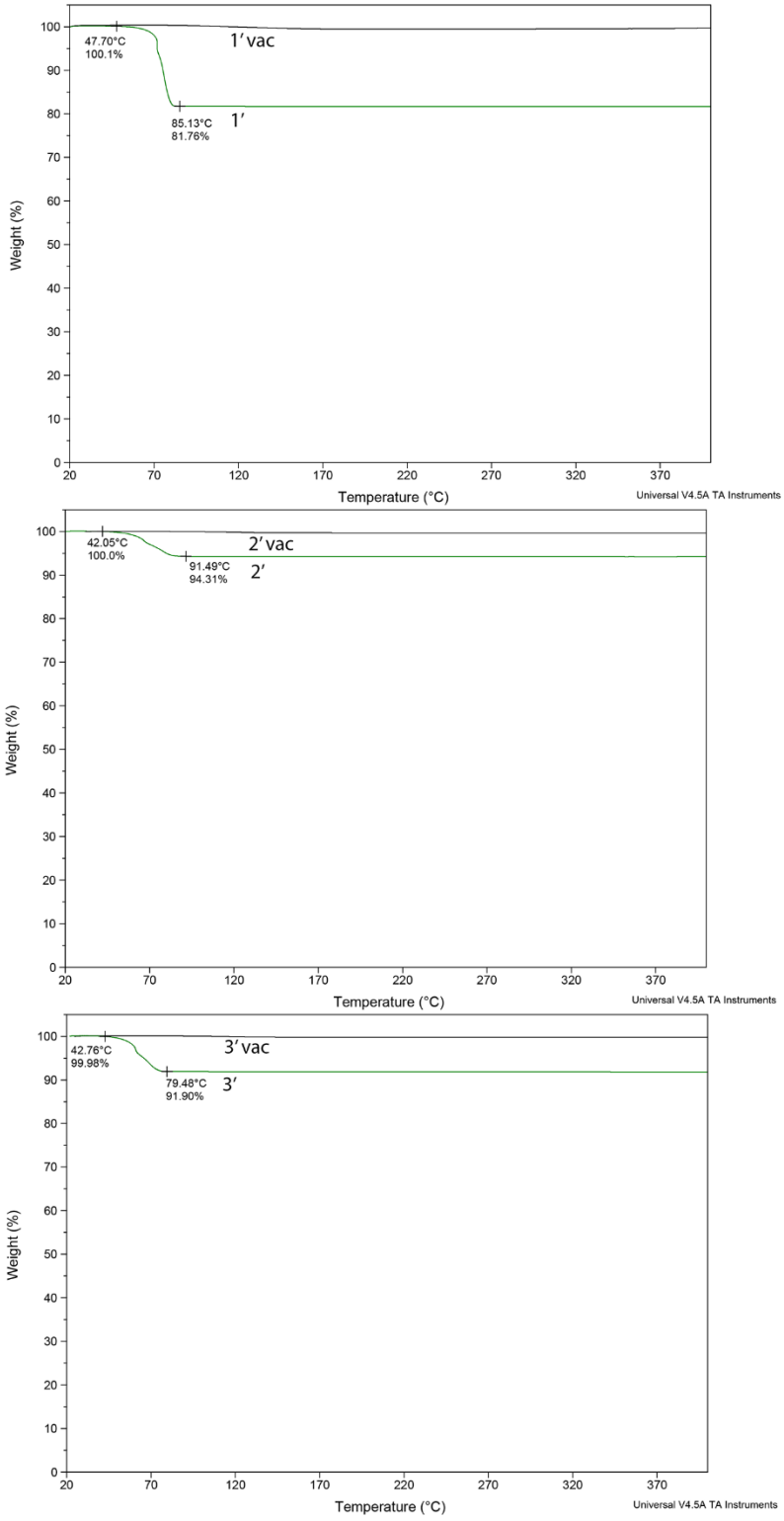

Figure S5. PXRD comparisons of **1′** before and after vacuum treatment (3 days, 100 μm vacuum).

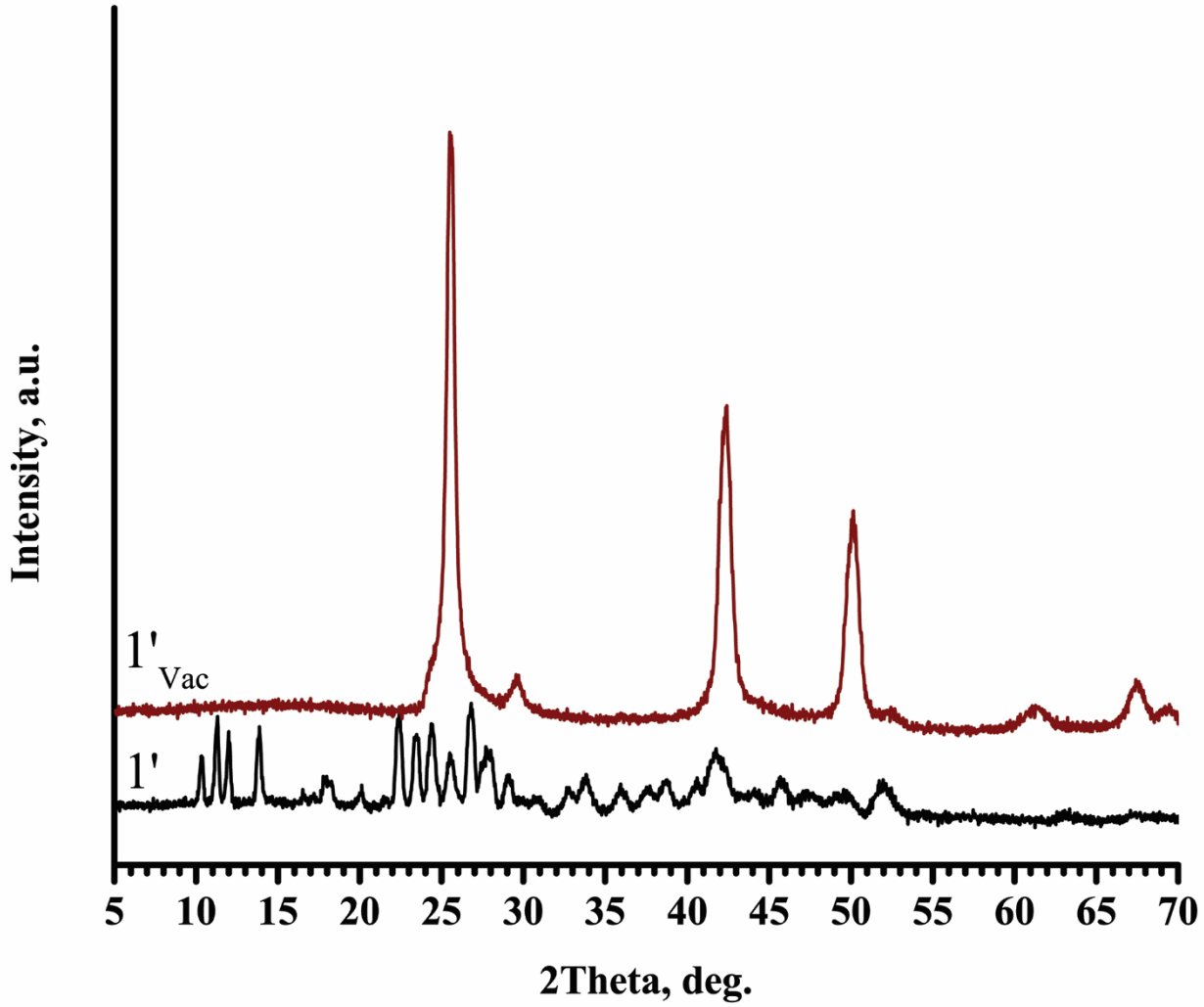

Figure S6. PXRD comparisons of **2′** before and after vacuum treatment (3 days, 100 μm vacuum).

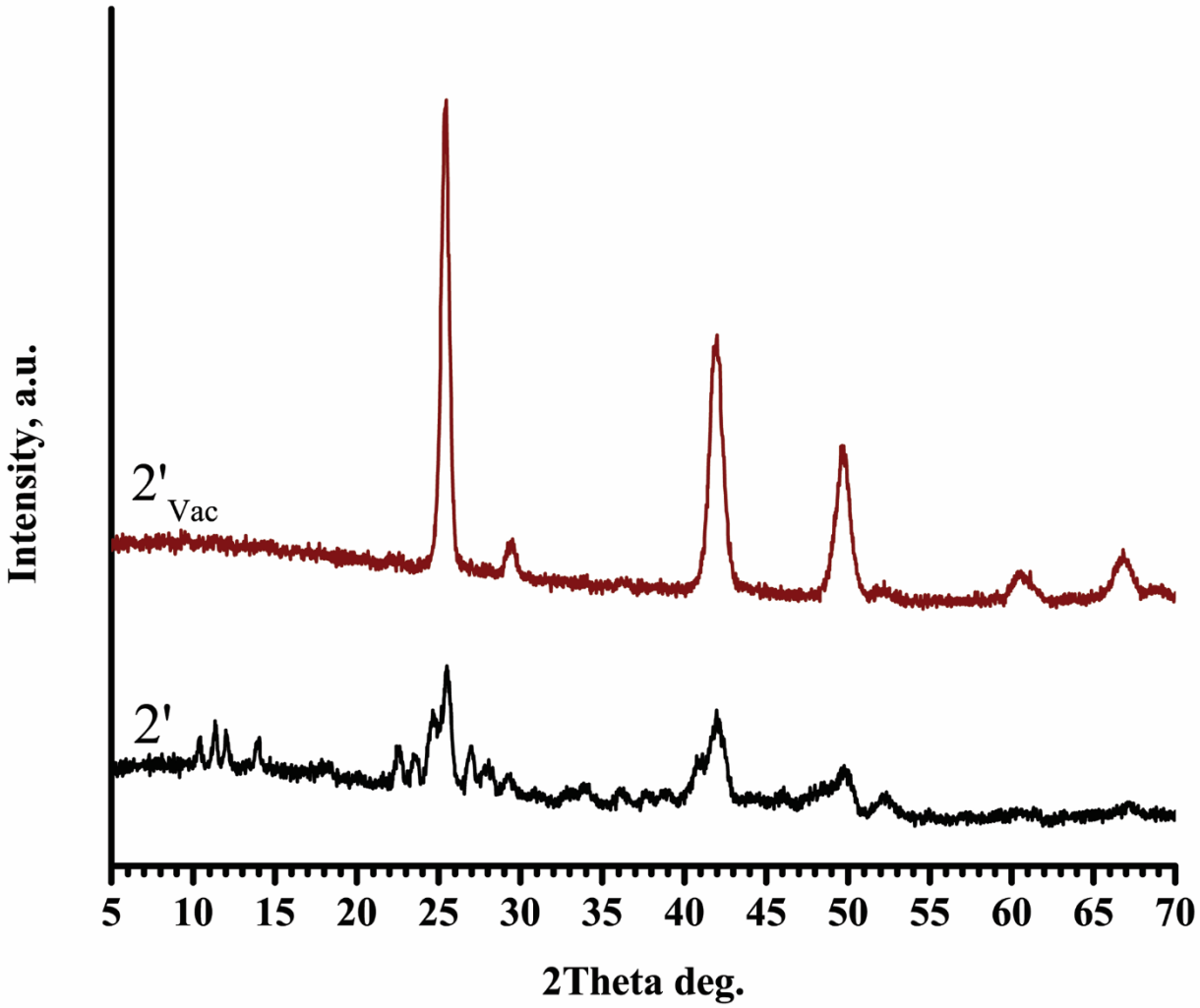

Figure S7. PXRD comparisons of **3′** before and after vacuum treatment (3 days, 100 μm vacuum).

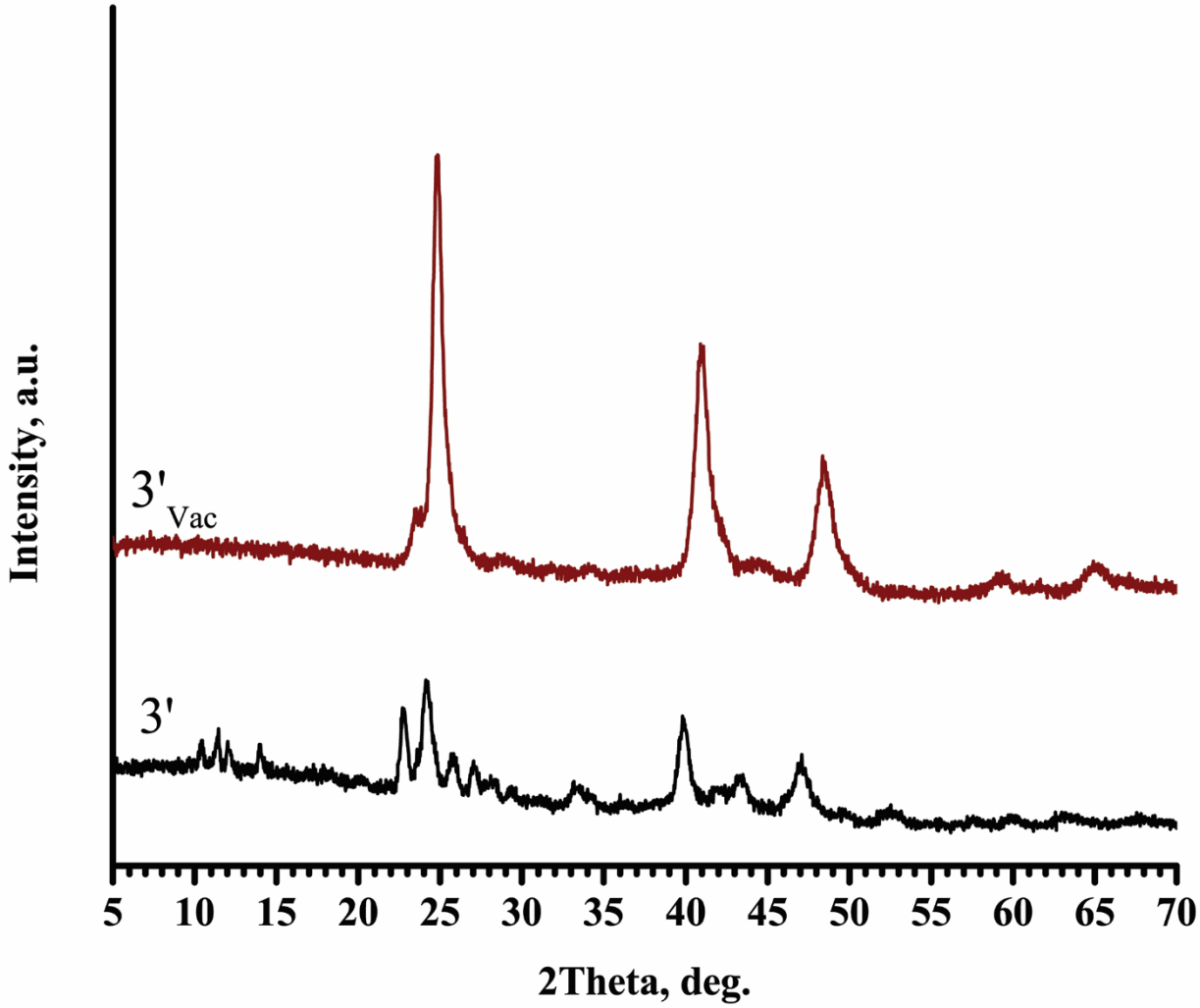

Figure S8. Luminescence photographs of **1′** after 0, 1, 2, 3, and 6 hours open bench exposure.

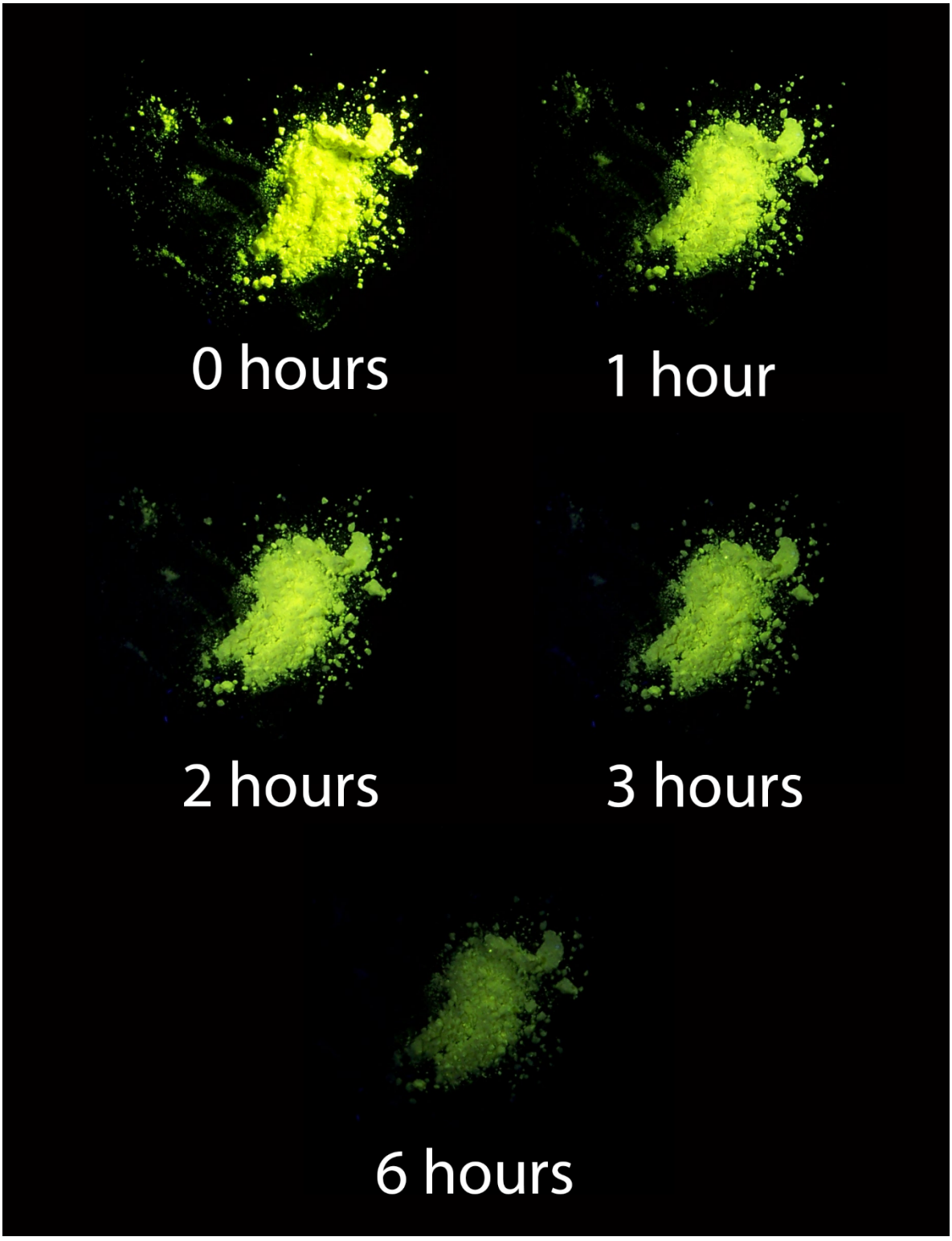

Figure S9. Solid state luminescence spectra of **1-3** and **1′-3′**. Note that **3** is non-emissive prior to exposure.

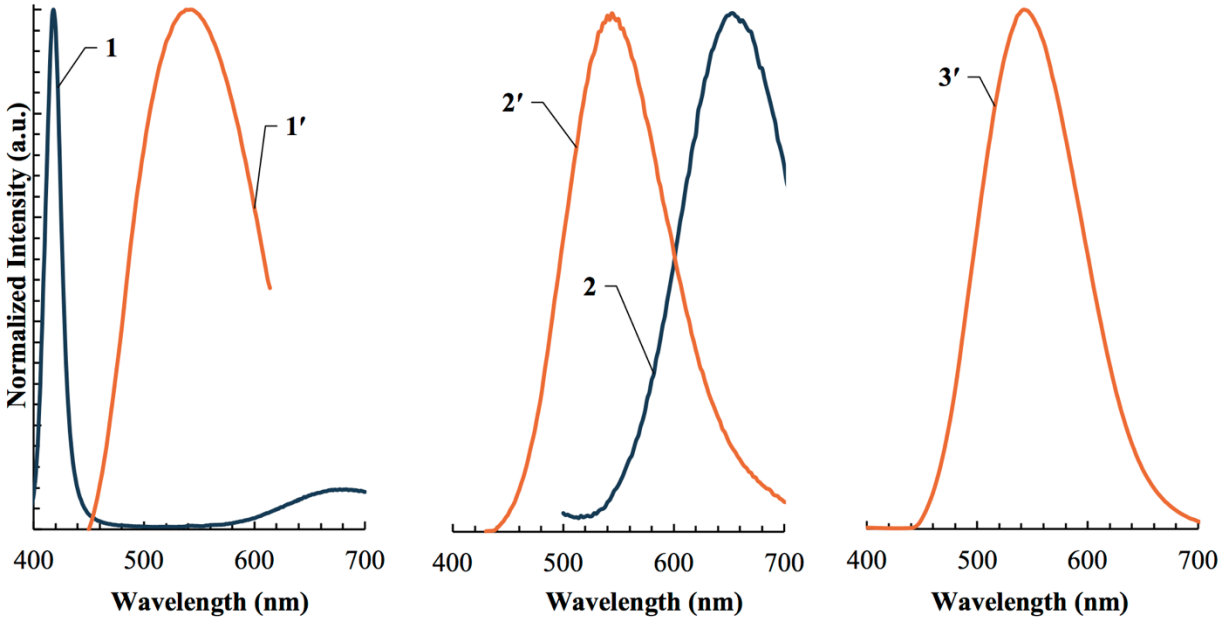

Figure S10. Wireframe packing diagram of $(CuI)_4DMS_3$ along the *a*-axis. Cu orange, I purple, S yellow, C gray, H white. Obtained from CSD 5.40 (Refcode: WEQLEK).[1]

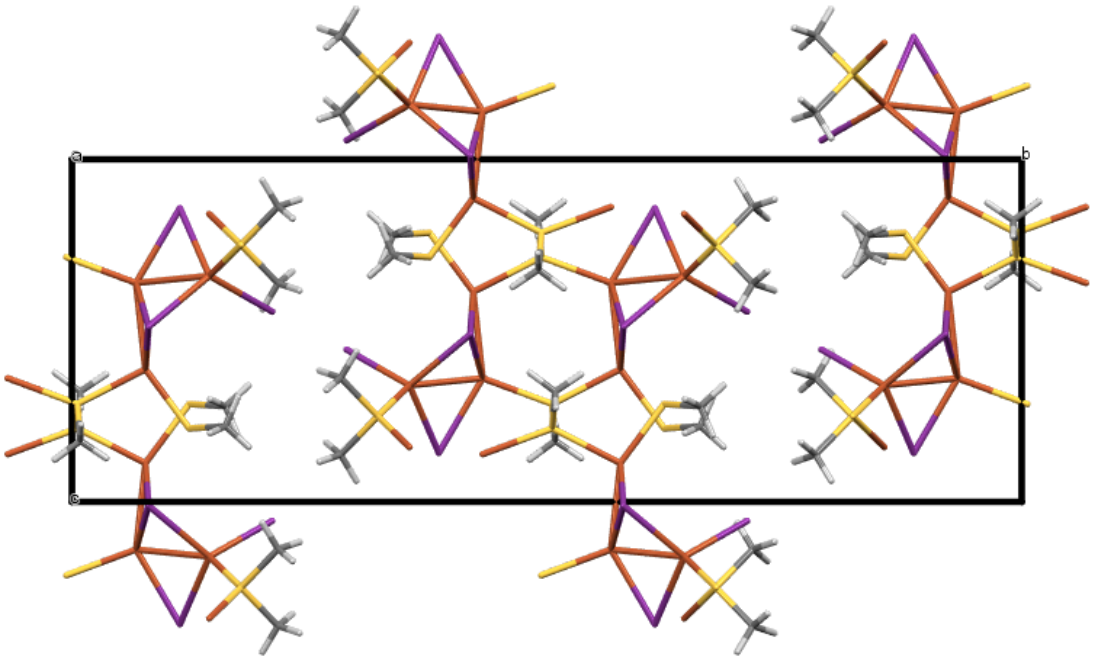

Figure S11. Wireframe packing diagram of $(CuI)_4DMS_3$ along the *c*-axis. Cu orange, I purple, S yellow, C gray, H white. Obtained from CSD 5.40 (Refcode: WEQLEK).[1]

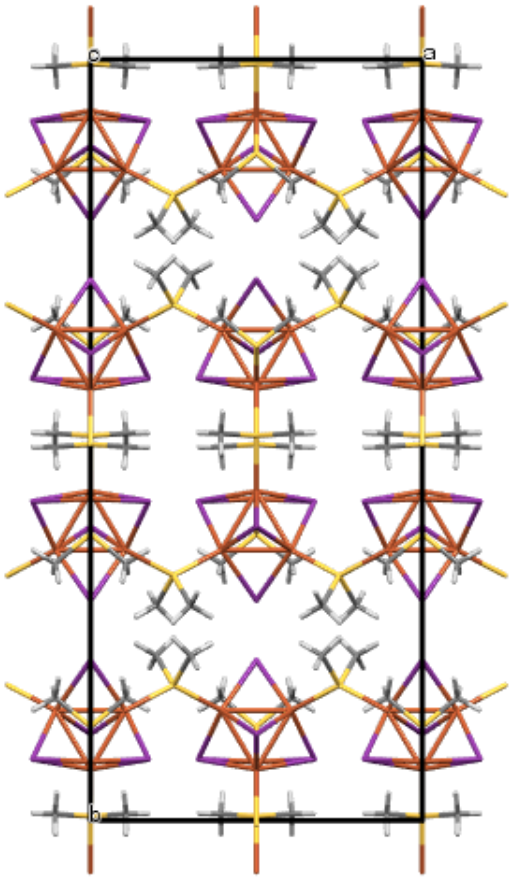

Figure S12. Offset FTIR spectra of DMS exposed nanoparticles **1′-3′**.

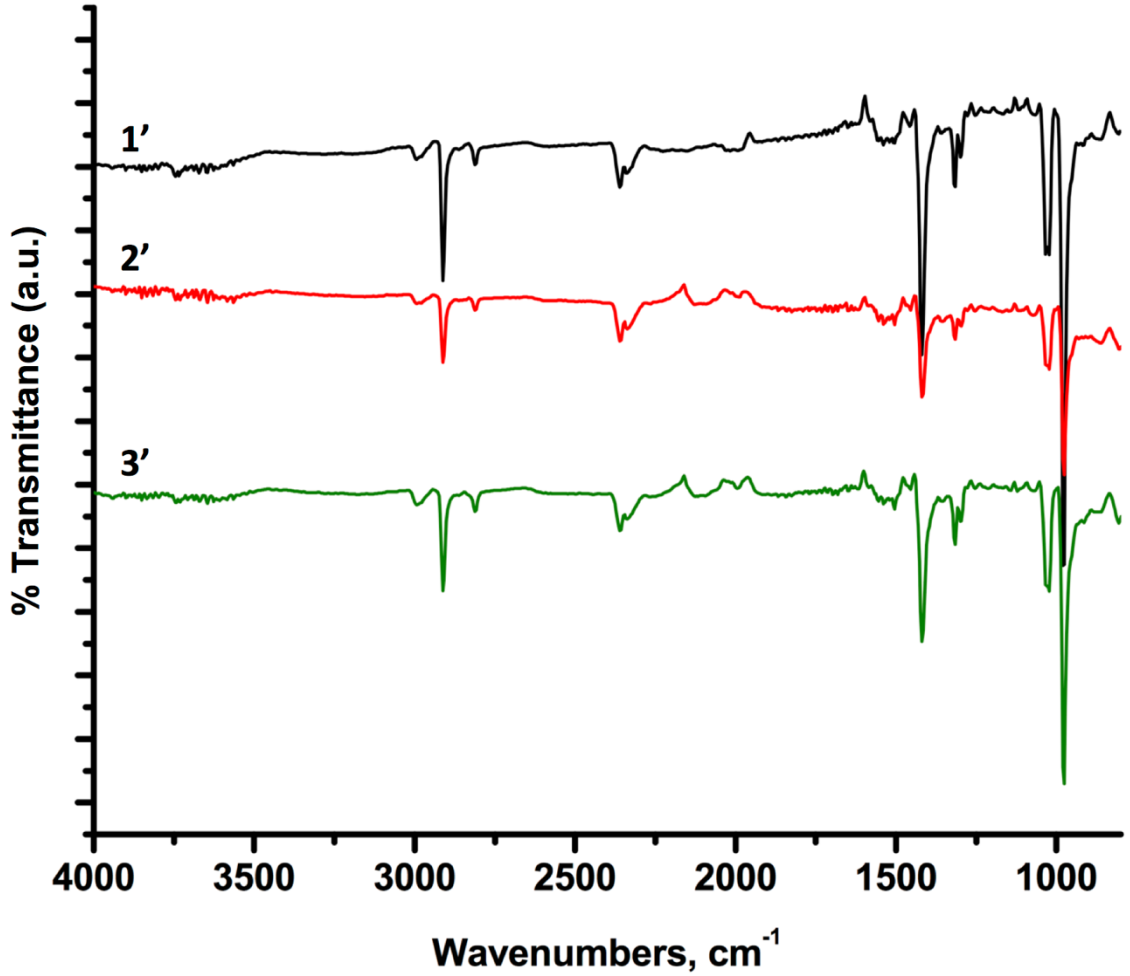

Figure S13. Offset FTIR spectra of DMS exposed nanoparticles **1′-3′** after vacuum treatment.

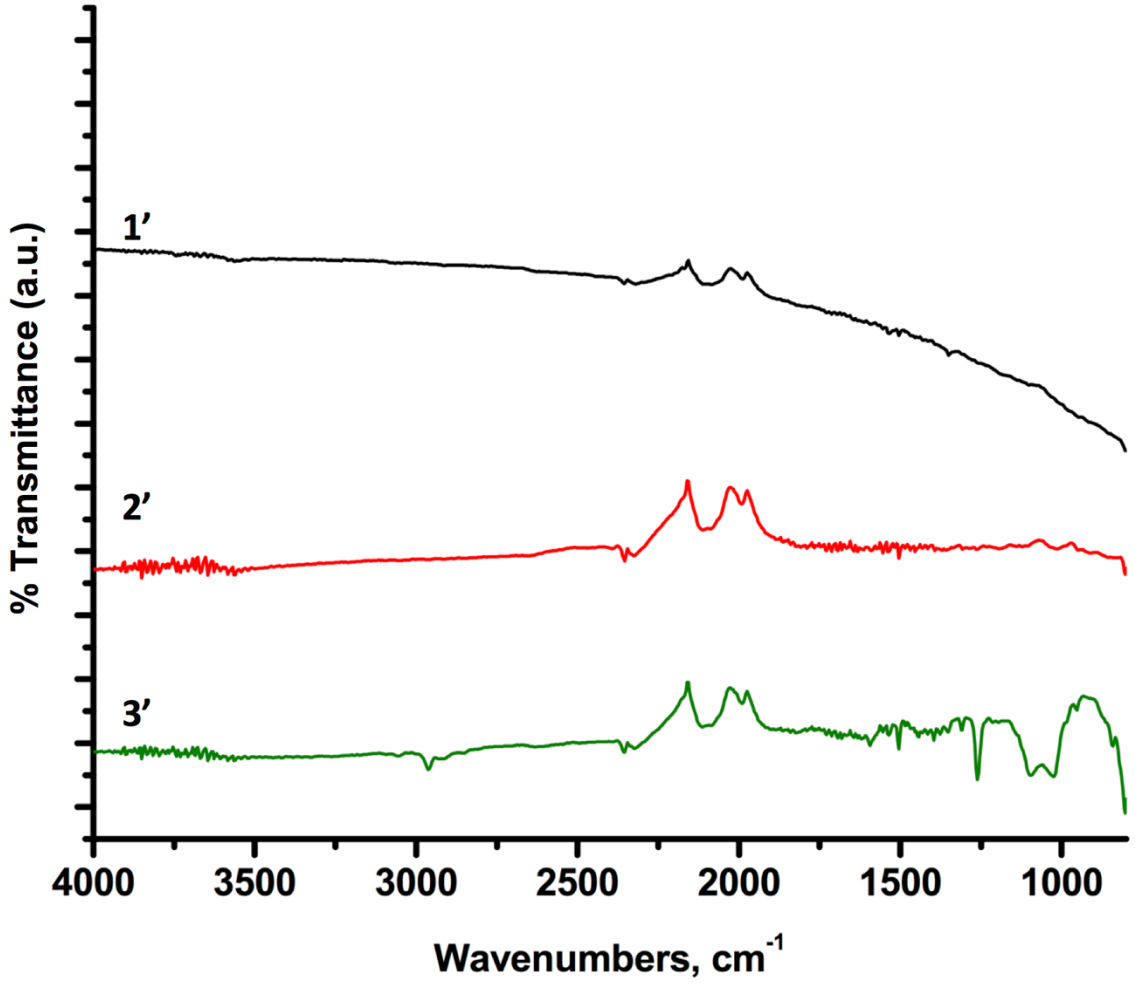

Figure S14. Additional TEM images of **1-3.**

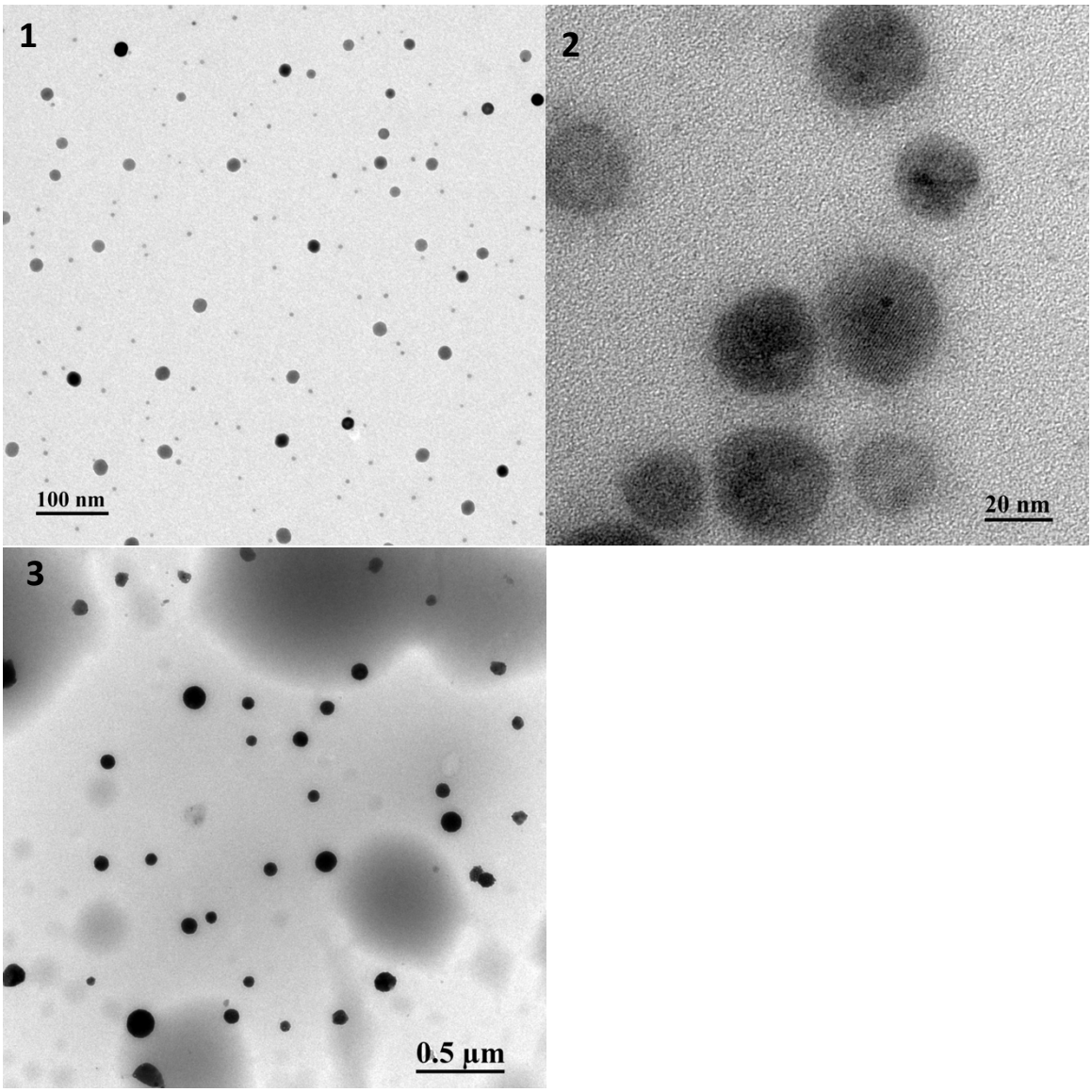

Table S1: Tables of Molecular Dynamic model parameters.

Atomic Charges

atom	charge
Ag	0.6
Cu	0.6
I	-0.6
C	0.22
S	-0.44

Lennard-Jones Parameters

atom 1	atom 2	ε (eV)	σ (Å)
Ag	S	0.05822	3.070
Ag	C	0.04215	3.141
Cu	S	0.05923	2.889
Cu	C	0.04288	2.956
I	S	0.009430	3.657
I	C	0.006830	3.736
S	S	0.01715	3.580
C	S	0.01241	3.663
C	C	0.008987	3.748

Vashishta-Rahman Parameters (form: Potential Energy = A/r^n)

atom 1	atom 2	A (eV)	n
Cu	I	186.811	7
Cu	I	-16.888	4
Ag	I	257.480	7
Ag	I	-16.888	4
I	I	5716.500	7
I	I	-33.776	4
I	I	-99.767	6

Simple Harmonic Stretch/Bend Parameters

atom 1	atom 2	atom 3	k (eV/Å^2 or eV/rad^2)	r_{equi}/θ_{equi} (Å or deg.)
C	S	--	19.7	1.82
S	C	C	5.38	99.0

References

(1) Knorr, M.; Bonnot, A.; Lapprand, A.; Khatyr, A.; Strohmann, C.; Kubicki, M. M.; Rousselin, Y.; Harvey, P. D. Reactivity of CuI and CuBr toward Dialkyl Sulfides RSR: From Discrete Molecular $Cu_4I_4S_4$ and $Cu_8I_8S_6$ Clusters to Luminescent Copper(I) Coordination Polymers. *Inorg. Chem.* **2015**, *54* (8), 4076–4093. https://doi.org/10.1021/acs.inorgchem.5b00327.