

Electronic Supplementary Information

Electron Transport Properties in Fluorinated Copper-Phthalocyanine Films: Importance of Vibrational Reorganization Energy and Molecular Microstructure

Fu-Chiao Wu,^a Horng-Long Cheng,^{*a} Chen-Hsiang Yen,^a Jyu-Wun Lin,^a Shyh-Jiun Liu,^b Wei-Yang Chou^a and Fu-Ching Tang^c

^a *Institute of Electro-Optical Science and Engineering,
Center for Micro/Nano Science and Technology,
Advanced Optoelectronic Technology Center,
National Cheng Kung University, Tainan 701, Taiwan, R.O.C.
E-mail: shlcheng@mail.ncku.edu.tw; Fax: +886 6 2095040 ;
Tel: +886 6 2757575 65286*

^b *Department of Material Science,
National University of Tainan, Tainan 700, Taiwan, R.O.C.*

^c *Department of Physics,
National Cheng Kung University
Tainan 701, Taiwan, R.O.C.*

1. Calculated Vibrational Reorganization Energy of F₁₆H₂Pc

Table S1. B3LYP/6-31G(d) calculations of frequencies and vibrational reorganization energies, λ_v , of A_g normal modes for F₁₆H₂Pc in its neutral state.

Calculated Frequency (cm ⁻¹)	λ_v	
	(meV)	(%)
103	2.73	2.25
161	0.02	0.02
271	0.05	0.04
271	0.07	0.06
313	0.46	0.38
326	0.09	0.07
436	0.48	0.39
462	0.24	0.20
568	0.88	0.73
722	8.27	6.84
743	9.01	7.45
947	22.76	18.81
969	4.01	3.31
1190	1.76	1.45
1334	0.05	0.04
1337	3.76	3.10
1381	0.18	0.15
1402	3.05	2.52
1441	21.04	17.38
1520	7.06	5.83
1524	0.33	0.27
1560	0.21	0.18
1617	0.86	0.71
1655	0.46	0.38
1668	33.08	27.34
3620	0.08	0.06
sum (meV) =	121.0	

2. Difference Spectrum between F₁₆CuPc thin-films grown on different substrate temperature

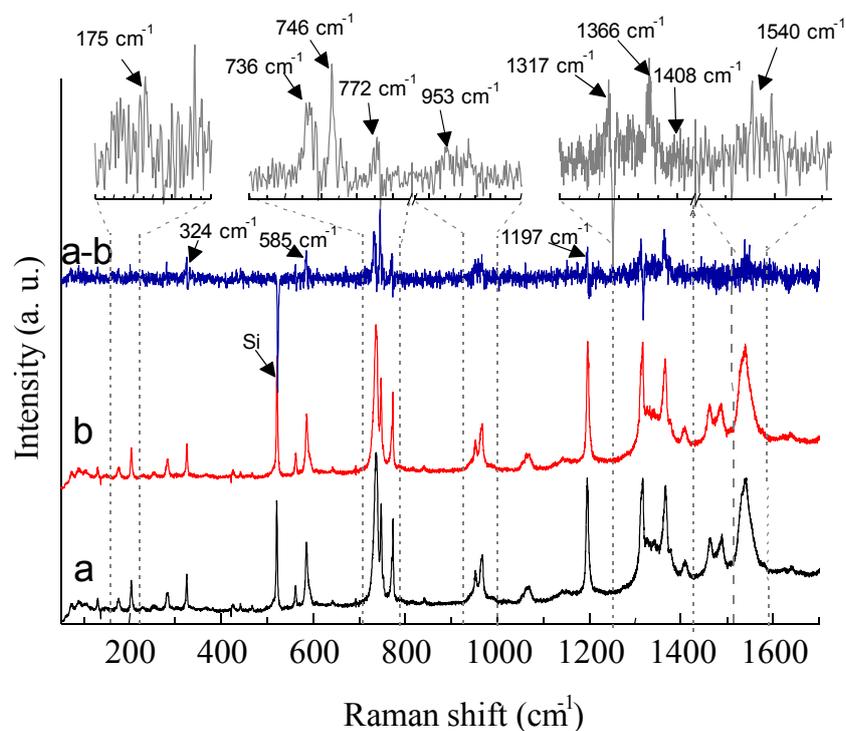


Fig. S1. Raman spectra ($\lambda_{exc} = 633$ nm) of F₁₆CuPc thin-films deposited at different substrate temperature: (a) 30 °C; (b) 120 °C. The spectra were normalized to the intensity of the 1540 cm⁻¹. Trace (a-b) is the difference spectrum, obtained by subtracting the spectra of (a) and (b). The bands discussed in the manuscript are labeled.

3. Polarized Raman spectrum

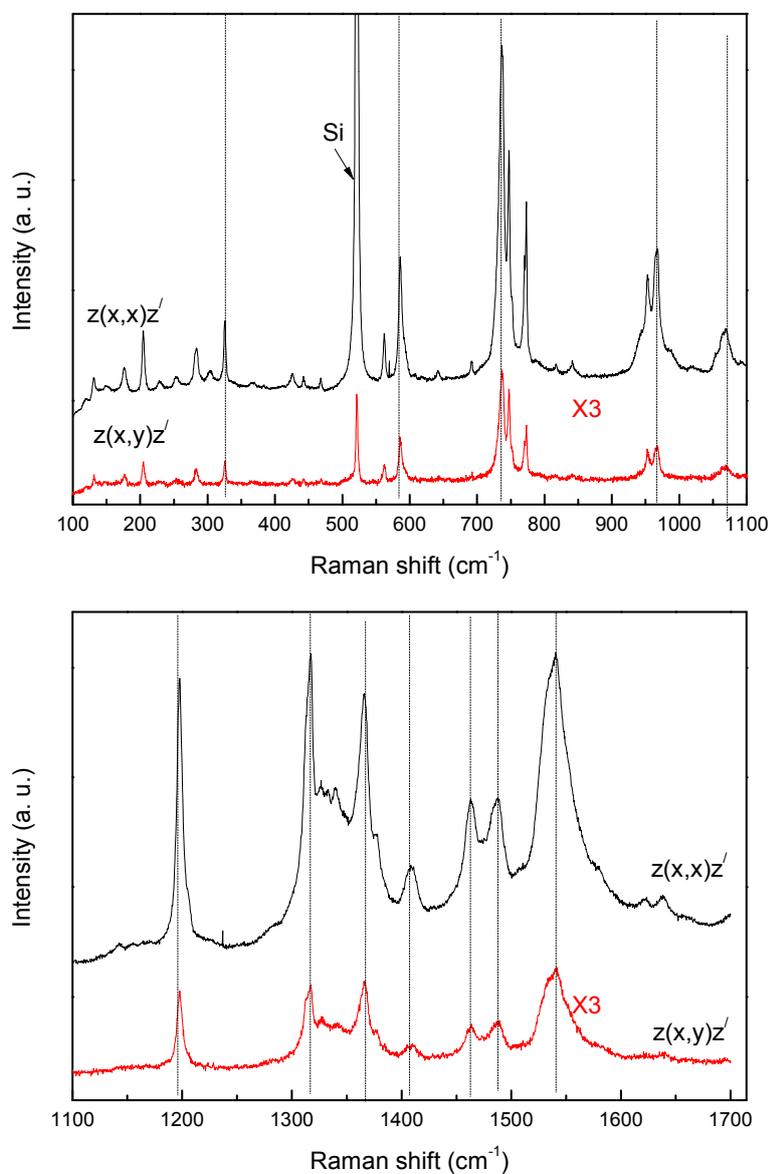


Fig. S2. Polarized Raman spectra ($\lambda_{exc} = 633$ nm) of the $F_{16}CuPc$ film. The polarizations of the incident and detected light are parallel (x,x) and perpendicular (x,y) to each other. The dashed lines serve as guidelines.