

Supporting Information

Microwave-assisted Synthesis of Novel Julolidinyl-Based Nonlinear Optical Chromophores with Enhanced Electro-optic Activity

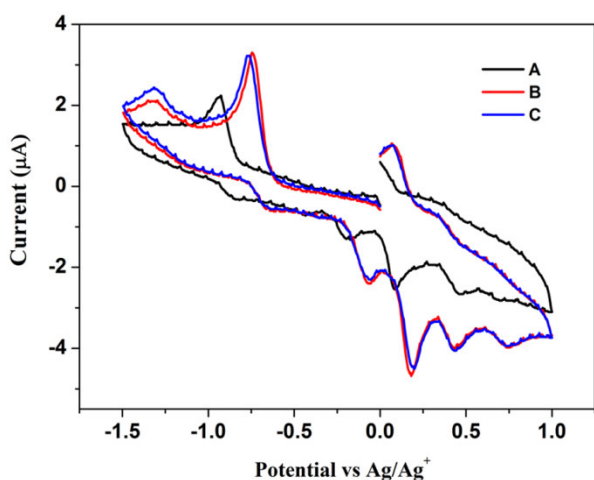
Airui Zhang,^{†,‡} Hongyan Xiao,[†] Chengcheng Peng,^{†,‡} Shuhui Bo,^{*,†} Guowei Deng,^{†,‡} Huajun Xu,^{†,‡}
Maolin Zhang,^{†,‡} Zhen Zhen,^{*,†} and Xinhou Liu[†]

[†]Key Laboratory of Photochemical Conversion and Optoelectronic Materials, Technique
Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing, 100190, PR China

[‡]University of Chinese Academy of Sciences, Beijing 100049, PR China

- 1. The redox potentials for three chromophores.**
- 2. Quantum mechanical calculations.**

- 1. Fig. S1 The redox potentials for chromophores A, B and C**



2. Quantum mechanical calculations.

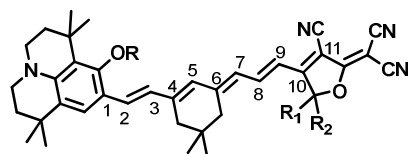


Fig. S2 Numbering of the carbon atoms in the conjugated bridge for chromophores A, B and C.

Cmpd	Sol	C ₁₋₂	C ₂₋₃	C ₃₋₄	C ₄₋₅	C ₅₋₆	C ₆₋₇	C ₇₋₈	C ₈₋₉	C ₉₋₁₀	C ₁₀₋₁₁	BLA
A	VC	1.448	1.370	1.438	1.382	1.427	1.388	1.415	1.383	1.415	1.398	-0.044
	DO	1.444	1.373	1.435	1.386	1.423	1.394	1.410	1.389	1.409	1.404	-0.035
	CF	1.441	1.376	1.431	1.391	1.418	1.400	1.404	1.395	1.403	1.411	-0.025
	DC	1.438	1.378	1.429	1.394	1.415	1.403	1.401	1.398	1.399	1.415	-0.019
	AC	1.436	1.380	1.427	1.396	1.413	1.406	1.399	1.401	1.396	1.418	-0.014
	AN	1.436	1.381	1.426	1.396	1.412	1.407	1.397	1.402	1.395	1.419	-0.012
B	VC	1.447	1.371	1.437	1.384	1.425	1.392	1.411	1.387	1.409	1.400	-0.039
	DO	1.441	1.376	1.431	1.391	1.417	1.400	1.403	1.395	1.400	1.409	-0.024
	CF	1.435	1.381	1.426	1.397	1.411	1.407	1.396	1.403	1.392	1.418	-0.011
	DC	1.432	1.384	1.422	1.401	1.407	1.412	1.392	1.407	1.388	1.423	-0.003
	AC	1.429	1.386	1.419	1.404	1.403	1.416	1.388	1.411	1.385	1.427	0.004
	AN	1.428	1.387	1.418	1.405	1.402	1.417	1.387	1.412	1.383	1.429	0.007
C	VC	1.447	1.371	1.437	1.384	1.425	1.392	1.411	1.387	1.409	1.400	-0.039
	DO	1.441	1.376	1.431	1.391	1.417	1.400	1.403	1.395	1.400	1.409	-0.024
	CF	1.435	1.381	1.426	1.397	1.411	1.407	1.396	1.403	1.393	1.417	-0.011
	DC	1.432	1.384	1.422	1.401	1.407	1.412	1.392	1.407	1.388	1.423	-0.003
	AC	1.429	1.386	1.419	1.404	1.403	1.416	1.388	1.411	1.385	1.427	0.004
	AN	1.428	1.387	1.418	1.406	1.402	1.417	1.387	1.412	1.383	1.429	0.007

[a]: VC: vacuum; DO: 1,4-dioxane; CF: chloroform; DC: dichloromethane; AC: acetone; AN: acetonitrile.