Electronic Supplementary Information for

Effects of changing substituents on the NLO properties of two coumarin derivatives

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Contents Page

Table ESI 1: MP2/6-311+G(d) results for the HOMO-LUMO for the compounds I.

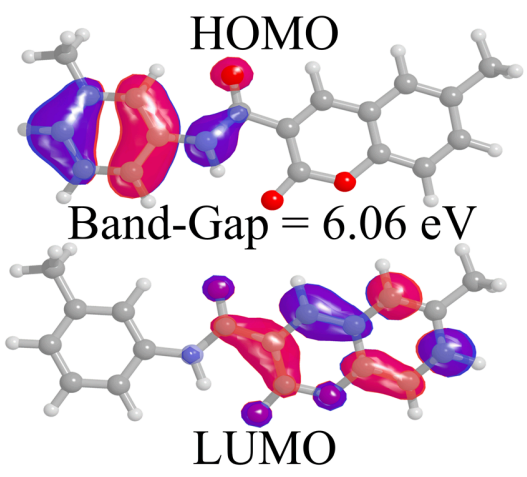
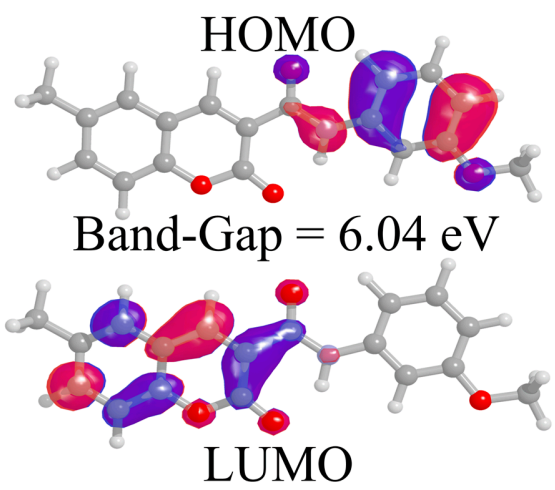
CH3	HOMO eV	LUMO eV
Acetone	-7.70	-1.57
Chloroform	-7.62	-1.56
Dichloromethane	-7.67	-1.56
DiMethylSulfoxide	-7.71	-1.57
Ethanol	-7.70	-1.57
Gas-Phase	-7.43	-1.58
Methanol	-7.71	-1.57
Water	-7.72	-1.57

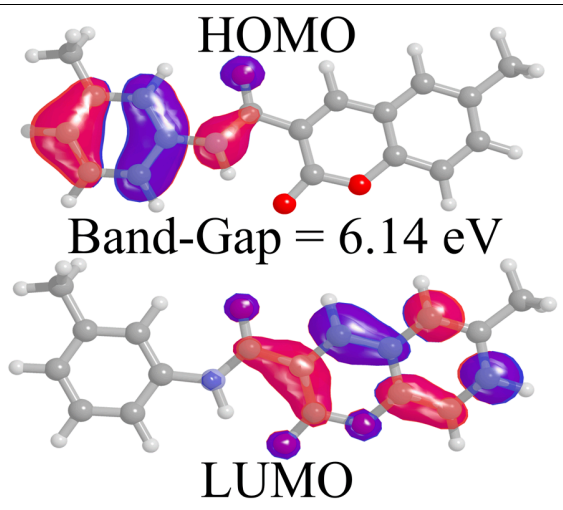
Table ESI 2: MP2/6-311+G(d) results for the HOMO-LUMO for the compounds I.

OCH3	HOMO eV	LUMO eV

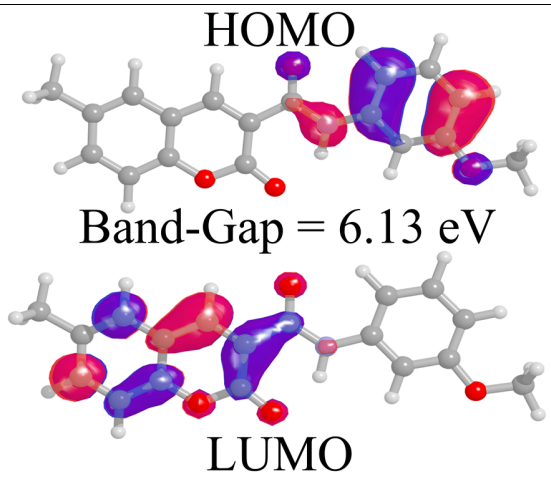
Acetone	-7.69	-1.57
Chloroform	-7.60	-1.56
Dichloromethane	-7.65	-1.57
DiMethylSulfoxide	-7.70	-1.57
Ethanol	-7.69	-1.57
Gas-Phase	-7.38	-1.57
Methanol	-7.70	-1.57
Water	-7.71	-1.57

Table ESI 3: The HOMO-LUMO frontiers orbitals for the coumarins compounds I and II in three different solvent media.

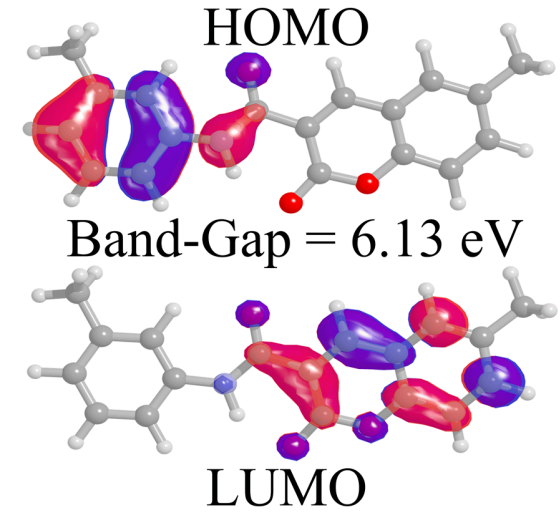
R21 (CH_3)	R22 (OCH_3)
Chloroform 	Chloroform 
DMSO	DMSO



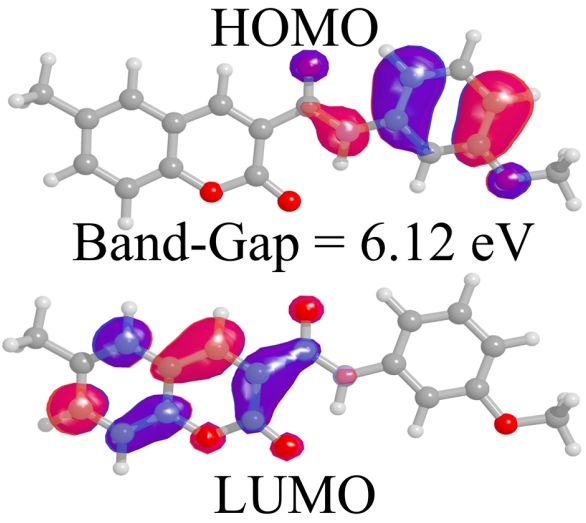
Ethanol



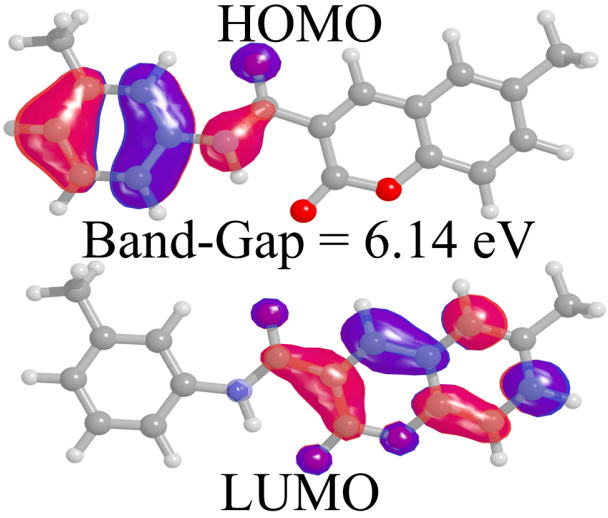
Ethanol



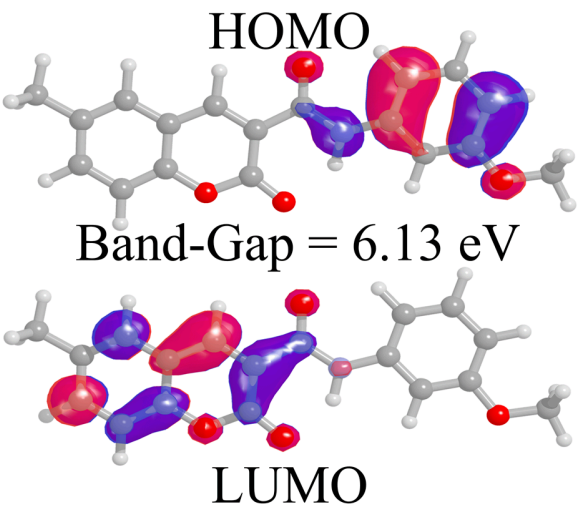
Methanol



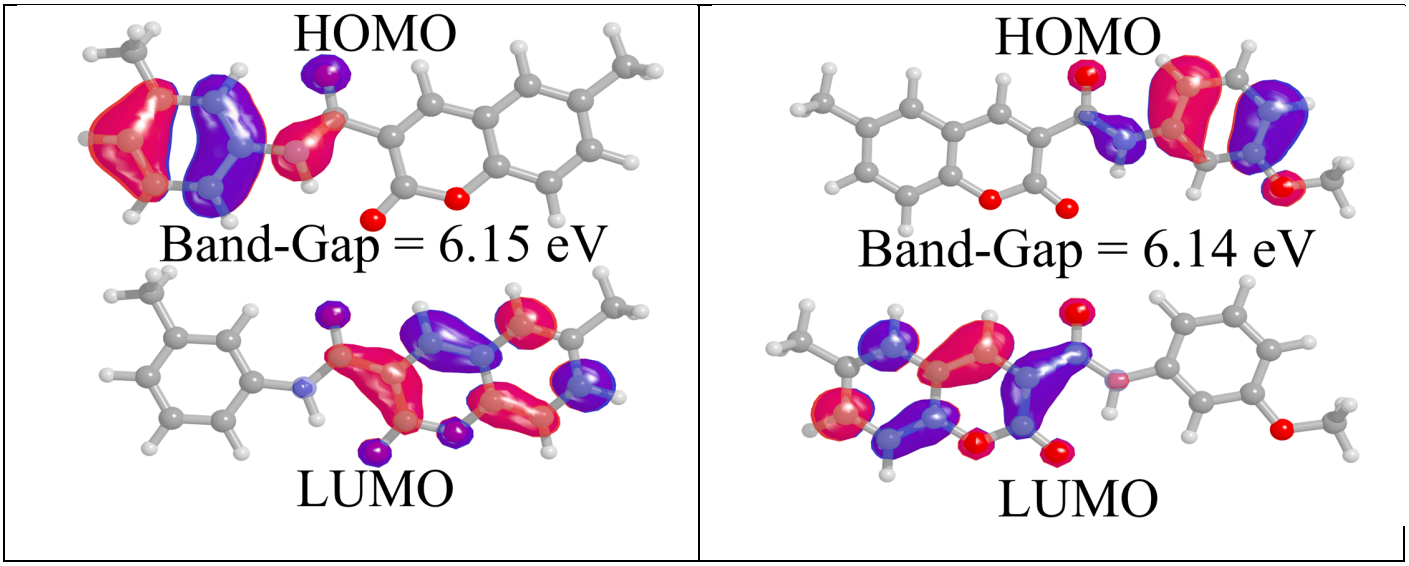
Methanol



Water



Water


HOMO
Band-Gap = 6.15 eV
LUMO
HOMO
Band-Gap = 6.14 eV
LUMO