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Band gap engineering of graphenylene by hydrogenation and halogenation: a density functional theory study

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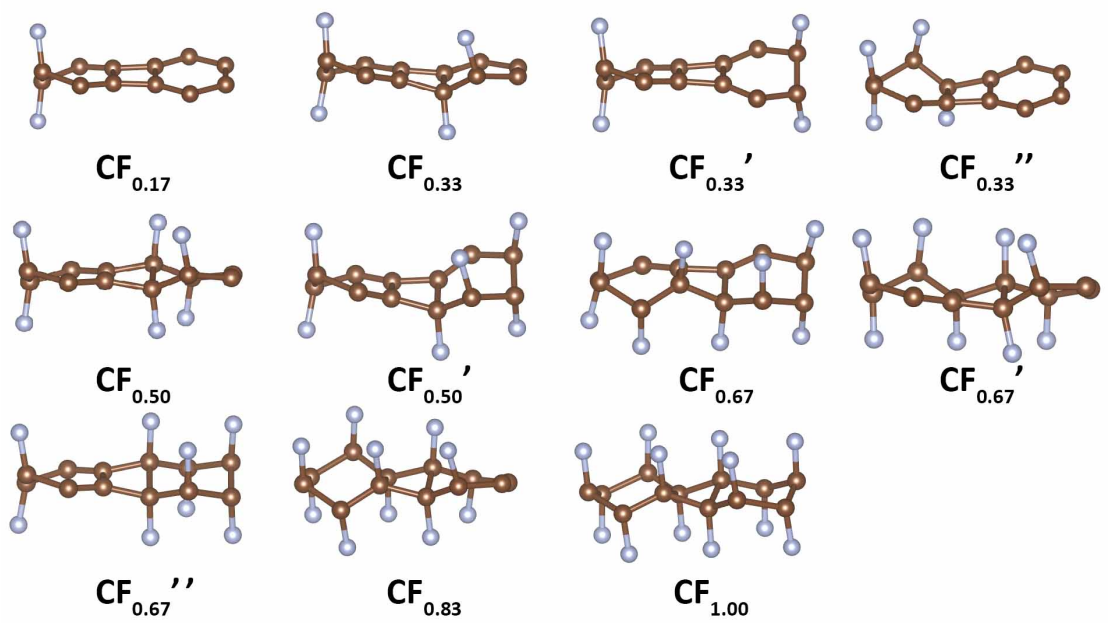

Figure S1. The structures of fluorinated graphenylene in one unit cell at various concentrations.

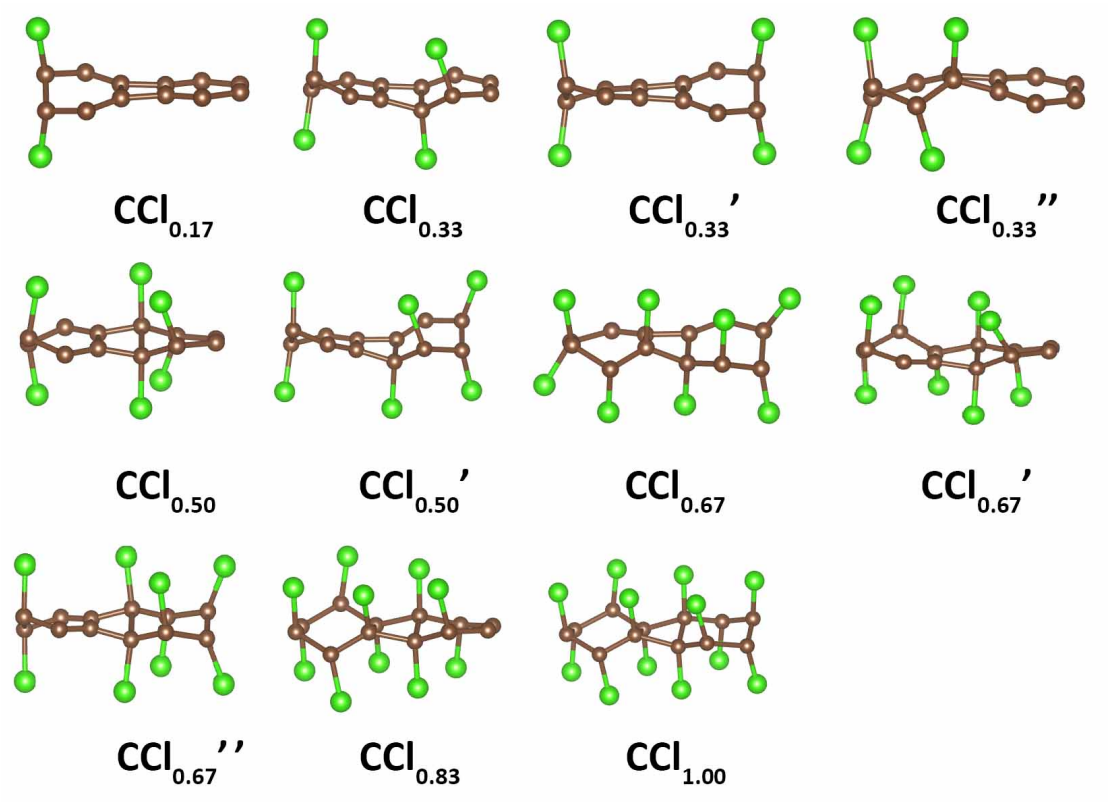

Figure S2. The structures of chlorinated graphenylene in one unit cell at various concentrations.

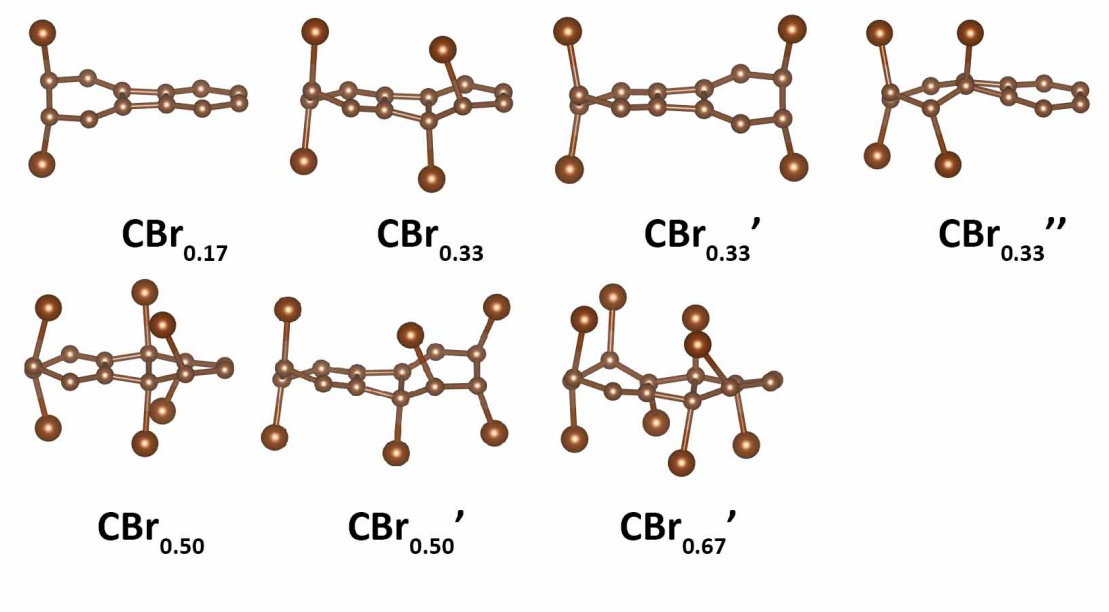

Figure S3. The structures of brominated graphenylene in one unit cell at various concentrations.

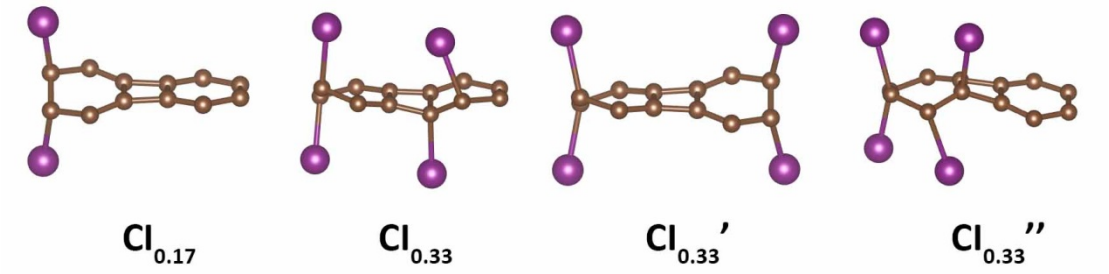

Figure S4. The structures of iodinated graphenylene in one unit cell at various concentrations.

Table S1. The calculated PBE energies of the obtained functionalized graphenylene. The unit of the values is eV.

	H	F	Cl	Br	I
$CX_{0.17}$	-110.402	-110.984	-107.296	-106.089	-105.068
$CX_{0.33}$	-117.831	-118.714	-110.751	-108.095	-105.726
$CX_{0.33}$'	-116.873	-117.915	-110.496	-108.093	-105.860
$CX_{0.33}$''	-117.680	-118.564	-110.524	-107.902	-105.491
$CX_{0.50}$	-125.136	-125.940	-112.055	-107.489	--
$CX_{0.50}$'	-124.775	-125.676	-113.382	-109.228	--
$CX_{0.67}$	-132.900	-133.587	-114.199	--	--
$CX_{0.67}$'	-132.893	-133.559	-114.205	-107.648	--
$CX_{0.67}$''	-132.544	-132.936	-113.969	--	--
$CX_{0.83}$	-140.779	-141.083	-114.573	--	--
$CX_{1.00}$	-148.592	-148.311	-114.974	--	--

Table S2. The calculated lattice constants of the obtained functionalized graphenylene. The unit of the values is Å.

	H	F	Cl	Br	I
$CX_{0.17}$	6.724	6.730	6.721	6.725	6.727
$CX_{0.33}$	6.639	6.657	6.623	6.648	6.671
$CX_{0.33}$'	6.669	6.656	6.662	6.673	6.700
$CX_{0.33}$''	6.796	6.709	6.689	6.734	6.751
$CX_{0.50}$	6.777	6.807	6.892	6.910	--
$CX_{0.50}$'	6.573	6.441	6.509	6.572	--
$CX_{0.67}$	6.755	6.818	6.944	--	--
$CX_{0.67}$'	6.751	6.808	6.948	6.958	--
$CX_{0.67}$''	6.792	6.841	6.956	--	--
$CX_{0.83}$	6.884	6.975	7.541	--	--
$CX_{1.00}$	6.940	7.045	7.725	--	--