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Structural, Mechanical, Electronic and Optical Properties of Biphenylene Hydrogenation: A First-Principles Study

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Supporting Information

The carbon-carbon band length of α, β and γ configurations numbered in Fig. 1 are shown in Table S1.

Table S1 The carbon-carbon band length of α, β and γ configurations

	Band length(Å)					
Biphenylene	d_1 = 1.448	d_2 = 1.407		d_3 = 1.457	d_4 = 1.456	
Configuration α	d_5 = 1.573	d_6 = 1.566		d_7 = 1.541	d_8 = 1.579	
Configuration β	d_9 = 1.574	d_{10} = 1.514	d_{11} = 1.557	d_{12} = 1.532	d_{13} = 1.591	d_{14} = 1.359
Configuration γ	d_{15} = 1.502	d_{16} = 1.500		d_{17} = 1.519	d_{18} = 1.541	

Refractive index n, extinction coefficient k, absorption coefficient α, transmittance T, reflectivity R, optical conductivity σ and energy-loss function L of α, β and γ configurations are plotted in Fig. S1.

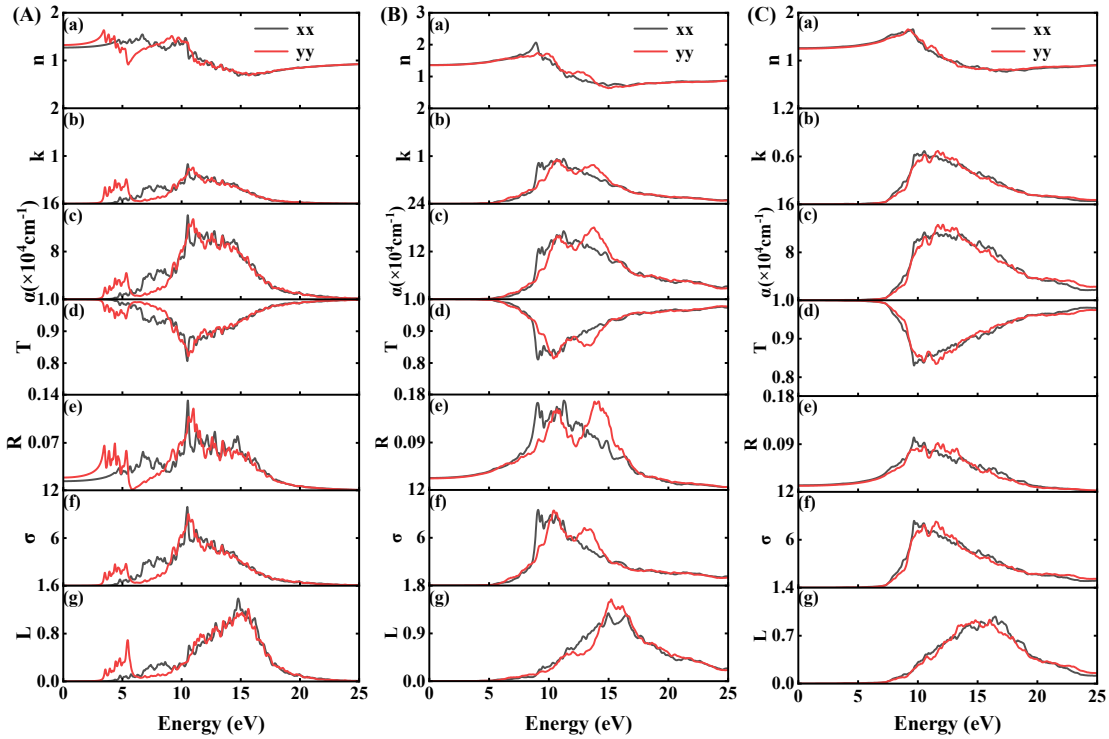

Fig. S1 The calculated optical properties of α (left panel), β (middle panel) and γ (right panel) configurations. There are two different directions of light polarization, xx and yy directions. (a) Refractive index *n*, (b) extinction coefficient *k*, (c) absorption coefficient *α*, (d) transmittance *T*, (e) reflectivity *R*, (f) optical conductivity *σ*, and (g) energy-loss function *L*.