Supplementary Materials

Research on the interaction mechanisms between $ScCO_2$ and low-rank / high-rank coal with ReaxFF-MD force field

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Table S1 Proximate and ultimate analyses of coal sample from YZ

$R_{o,max}$(%)	Promximate analysis (%)			Ultimate analysis (%)				
	M_{ad}	A_{ad}	V_{daf}	C	H	O	N	S
0.62	1.92	14.32	46.23	80.17	5.61	8.12	1.43	4.68

Table S2 Proximate and ultimate analyses of coal sample from CZ

$R_{o,max}$(%)	Promximate analysis (%)			Ultimate analysis (%)				
	M_{ad}	A_{ad}	V_{daf}	C	H	O	N	S
3.21	0.74	14.76	11.3	89.22	3.51	1.10	0.56	4.68

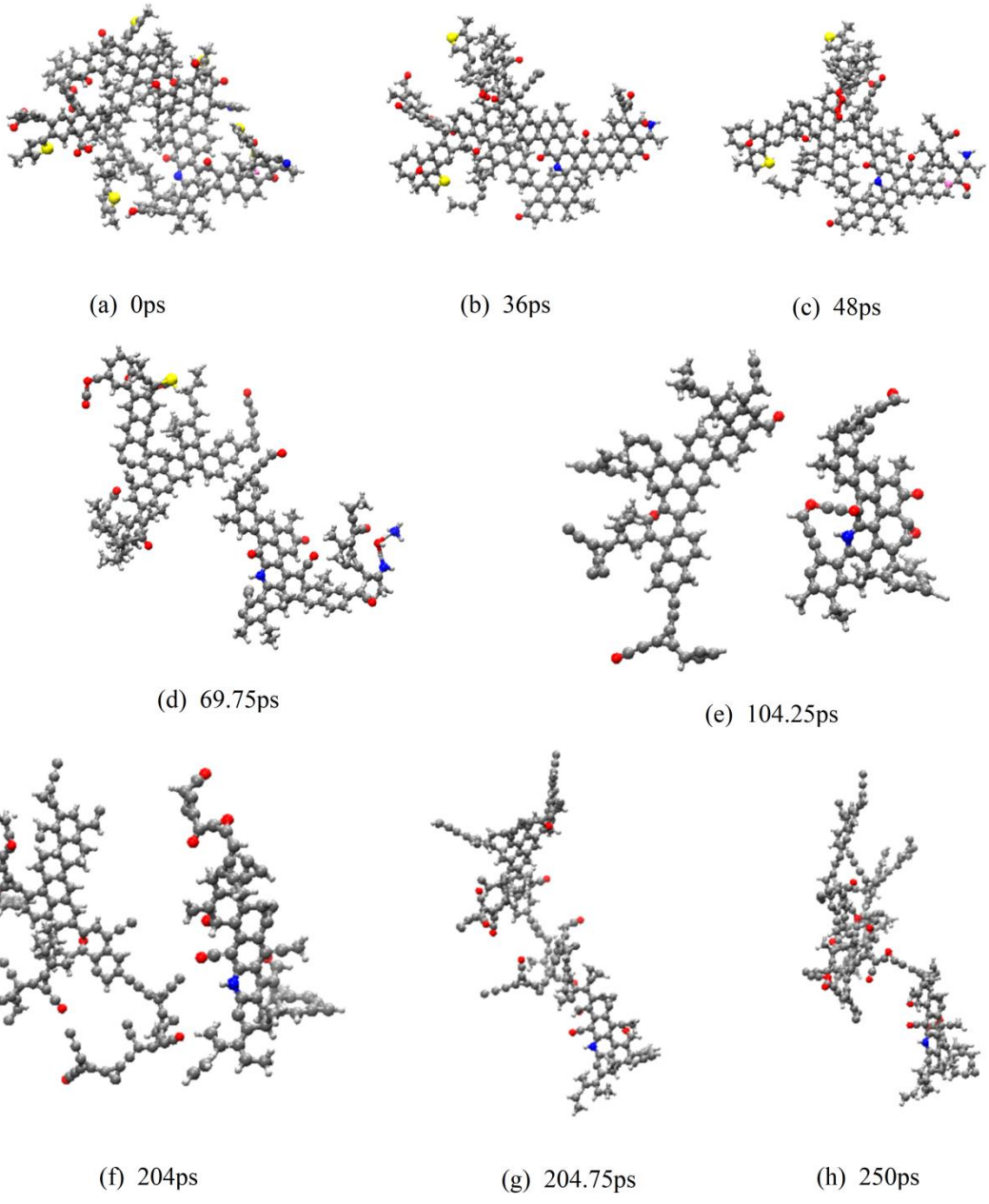

Figure S1. The low-rank coal macromolecular structures reaction process with $ScCO_2$

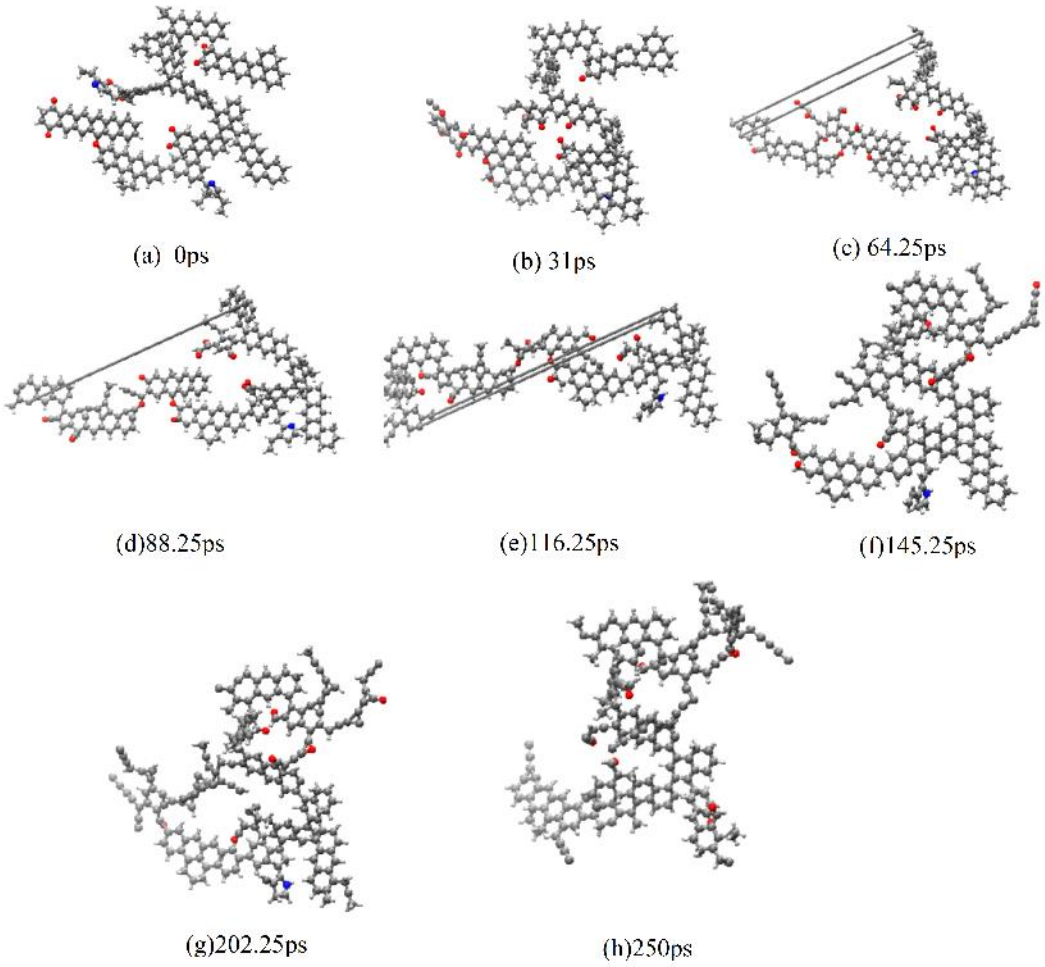

Figure S2. The high-rank coal macromolecular structures reaction process with $ScCO_2$