Electronic Supplementary Material (ESI) for RSC Advances.
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Table 1 The main bond parameters of oxetane and its protonated ion(bond length: nm, bond angle: °)

	Ox					$Ox-H^+$				
Bond parameters	C1C2	C2O3	C1C2O3	C2C1C4	C2O3C4	C1C2	C2O3	C1C2O3	C2C1C4	C2O3C4
B3LYP/6-31G(d,p)	0.154	0.145	91.95	84.49	91.62	0.153	0.154	89.29	89.55	89.31
B3LYP/6-311++G(d,p)	0.154	0.145	91.76	84.77	91.71	0.153	0.154	89.28	89.75	89.23
MP2/6-31G(d,p)	0.153	0.145	92.09	84.74	91.08	0.153	0.153	88.64	89.02	88.62
MP2/6-311++G(d,p)	0.154	0.145	92.24	84.39	91.14	0.153	0.153	88.72	88.45	88.70
Experiment	0.155	0.145	91.91	84.61						

Table 2 the atomic charge of oxetane and its protonated cation with the basis of 6-31G(d,p)

	method	O	C	C	C	H	H	H	H	H	H	H
Ox	Mulliken	-0.514	0.094	0.094	-0.282	0.112	0.112	0.096	0.096	0.096	0.096	
	Becke	-0.194	-0.269	-0.269	-0.343	0.181	0.181	0.178	0.178	0.178	0.178	
	Hirshfield	-0.199	0.041	0.041	-0.045	0.030	0.030	0.026	0.026	0.026	0.026	
	ADCH	-0.287	-0.026	-0.026	-0.146	0.087	0.087	0.078	0.078	0.078	0.078	
Ox-H+	Mulliken	-0.437	0.023	0.023	-0.278	0.201	0.202	0.206	0.225	0.225	0.206	0.405
	Becke	-0.070	-0.201	-0.201	-0.305	0.227	0.227	0.234	0.242	0.242	0.234	0.372
	Hirshfield	0.032	0.120	0.120	-0.006	0.074	0.072	0.082	0.088	0.088	0.082	0.248
	ADCH	-0.221	-0.013	-0.013	-0.151	0.153	0.149	0.159	0.171	0.171	0.159	0.434

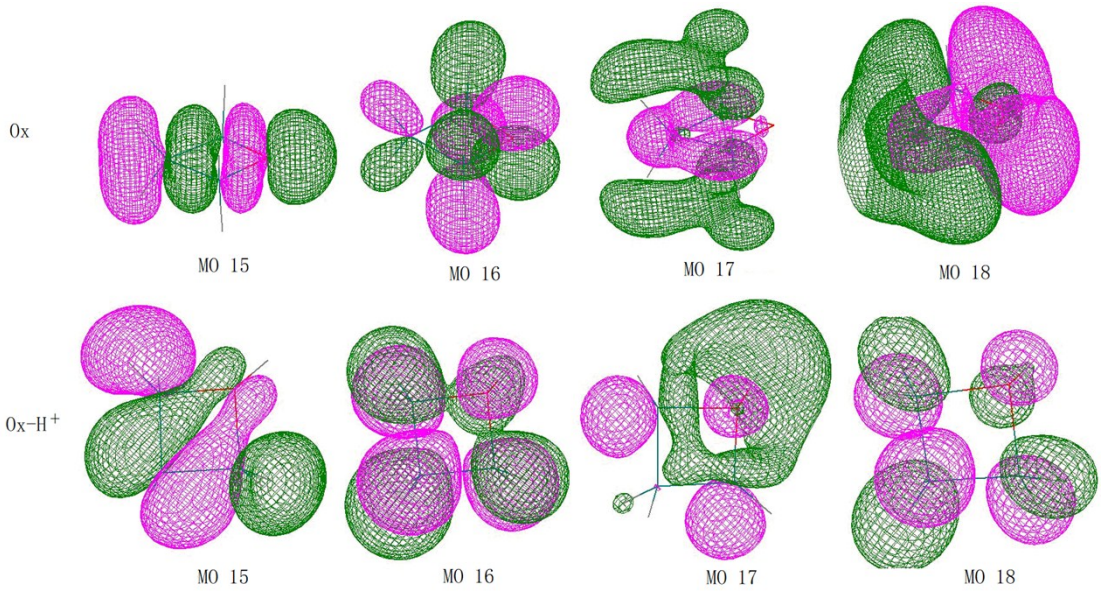
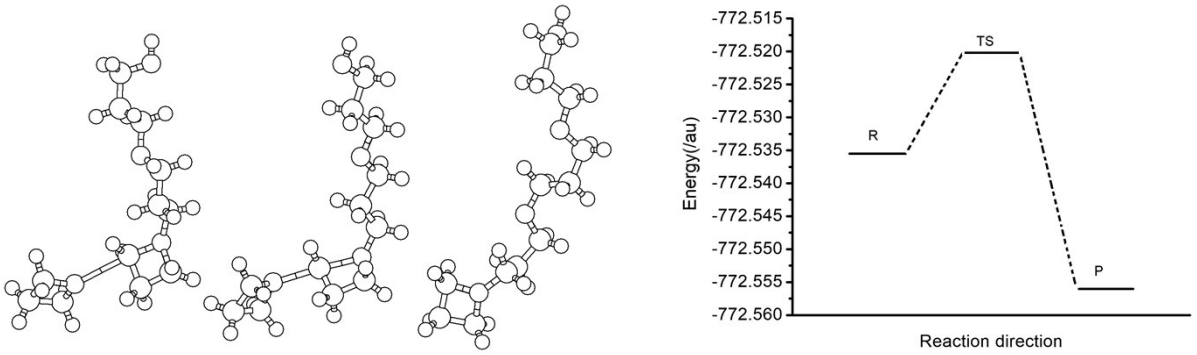
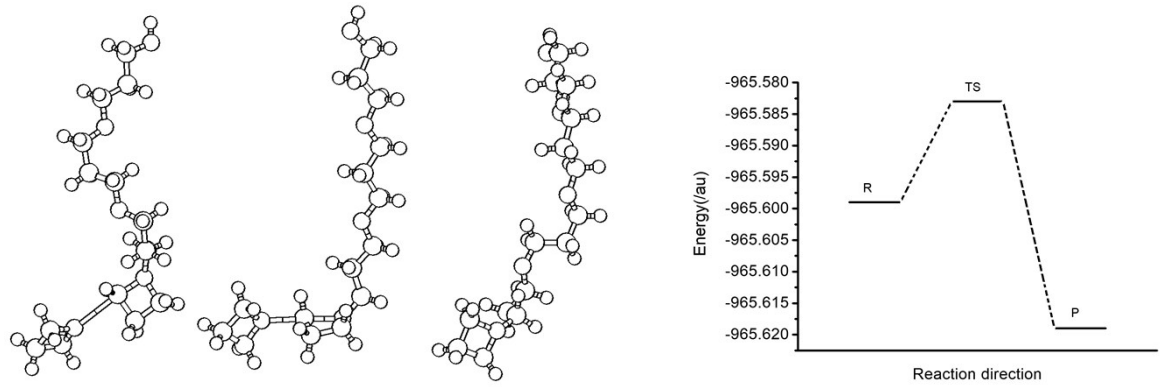


Figure 1 MO15, 16(HOMO); MO17,18(LUMO) of the frontier molecular orbital of oxetane molecule and its protonated ion



(a) four-polymerization



(b) five-polymerization

Figure 2 Structural models of reactant, transition state and product of oxetane 4- and 5-polymerization