

Supplementary materials

Figure

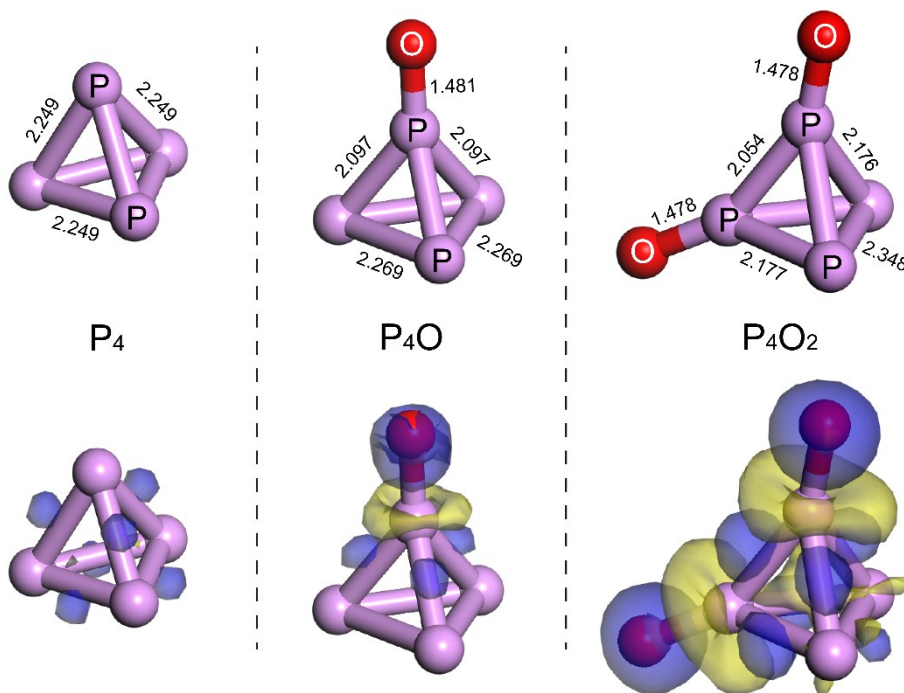


Fig. S1 Bond length and charge density of P_4 , P_4O and P_4O_2 (Bond length in Å)

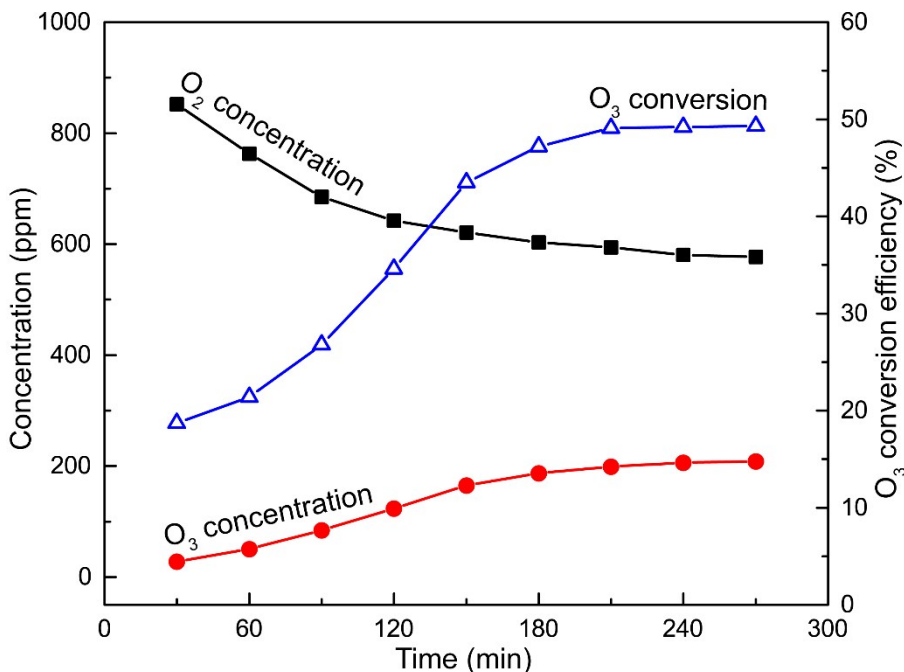


Fig. S2 Static experiment for O_3 generation over P_4 (Reaction conditions: reaction temperature = 25 °C; gas hourly space velocity = 1000 h^{-1} ; balanced gas = N_2 , initial O_2 = 1000 ppm)

Tables

Table S1 Imaginary frequencies of the transition states and bonds corresponding to relative normal vibrations for ozone generation without the involvement of H₂O

Transition States	Imaginary frequency (cm ⁻¹)	Bonds corresponding to relative normal vibrations
TS1	-1429.07	O5-O6
TS2	-1022.86	O6-O7
TS3	-1307.51	O5-P1
TS4	-1148.19	O11-O12
TS5	-989.43	O12-O13

Table S2 Imaginary frequency of the transition states and bonds corresponding to relative normal vibrations for ozone generation with the involvement of H₂O

Transition States	Imaginary frequency (cm ⁻¹)	Bonds corresponding to relative normal vibrations
TS6	-857.35	H8-O7
TS7	-1207.69	H8-O6
TS8	-785.32	O6-O10