

Fig. S1 Configuration of methane-oxygen system with 10 mol% water addition added in at 700 ps, (white, gray and red balls denote hydrogen atoms, carbon atoms and oxygen atoms, respectively. This is the same as the following figures).

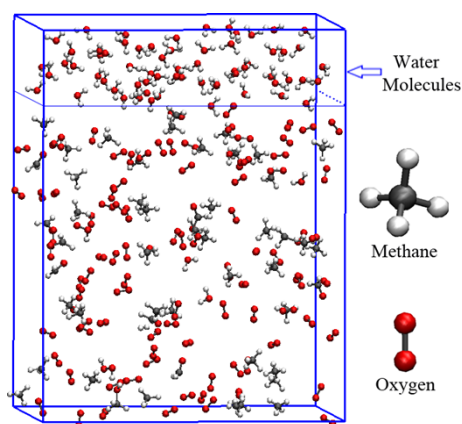


Fig. S2 Configuration of methane-oxygen system with 30 mol% water addition added in at 700 ps.

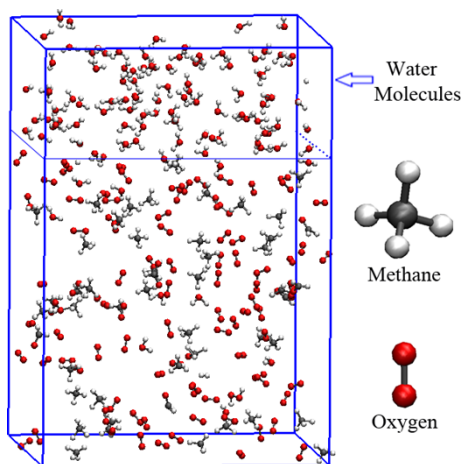


Fig. S3 Configuration of methane-oxygen system with 40 mol% water addition added in at 700 ps.

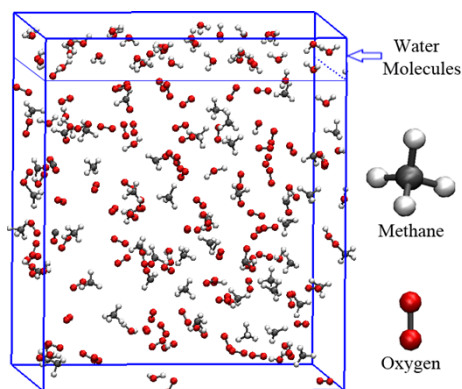


Fig. S4 Configuration of methane-oxygen system with 20 mol% water addition added in at 800 ps.

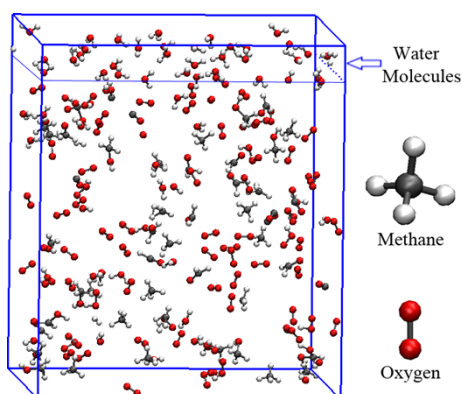


Fig. S5 Configuration of methane-oxygen system with 20 mol% water addition added in at 900 ps.

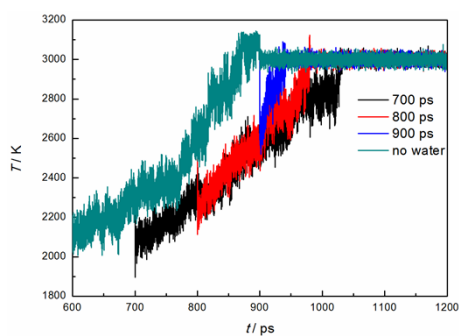


Fig. S6 Changes of system temperature when 20 mol% water addition is added in at the different reaction stages (700, 800 and 900ps).

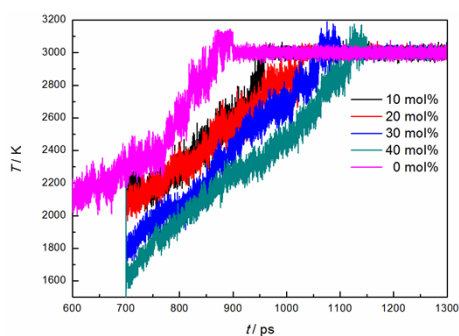


Fig. S7 Changes of system temperature with water addition mole fractions from 0 to 40 mol%.