

Supporting Information

Table S1. Self-diffusion coefficients of propylene in one and three dimensions

	D_s	D_x	D_y	D_z
System 1	1.8387	2.37955	2.65249	0.48405
System 2	2.61355	3.43277	3.11402	1.29386
System 3	3.76683	6.33421	4.40895	0.55731
System 4	4.87606	5.66039	7.61823	1.34957
System 5	5.50115	7.03339	7.66663	1.80343
System 6	5.99429	6.16076	9.94255	1.87957

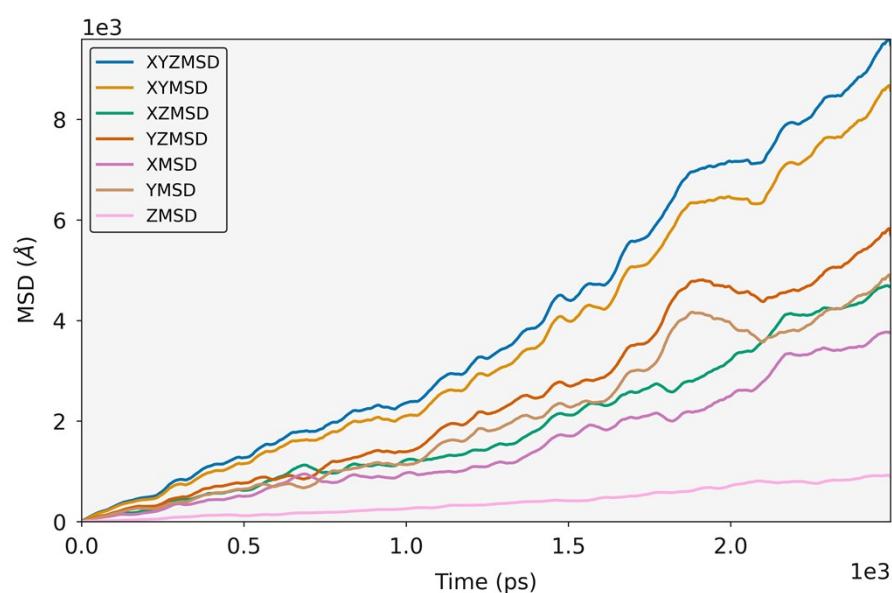


Figure S1 MSD of propylene in one and two dimensions in system 6.

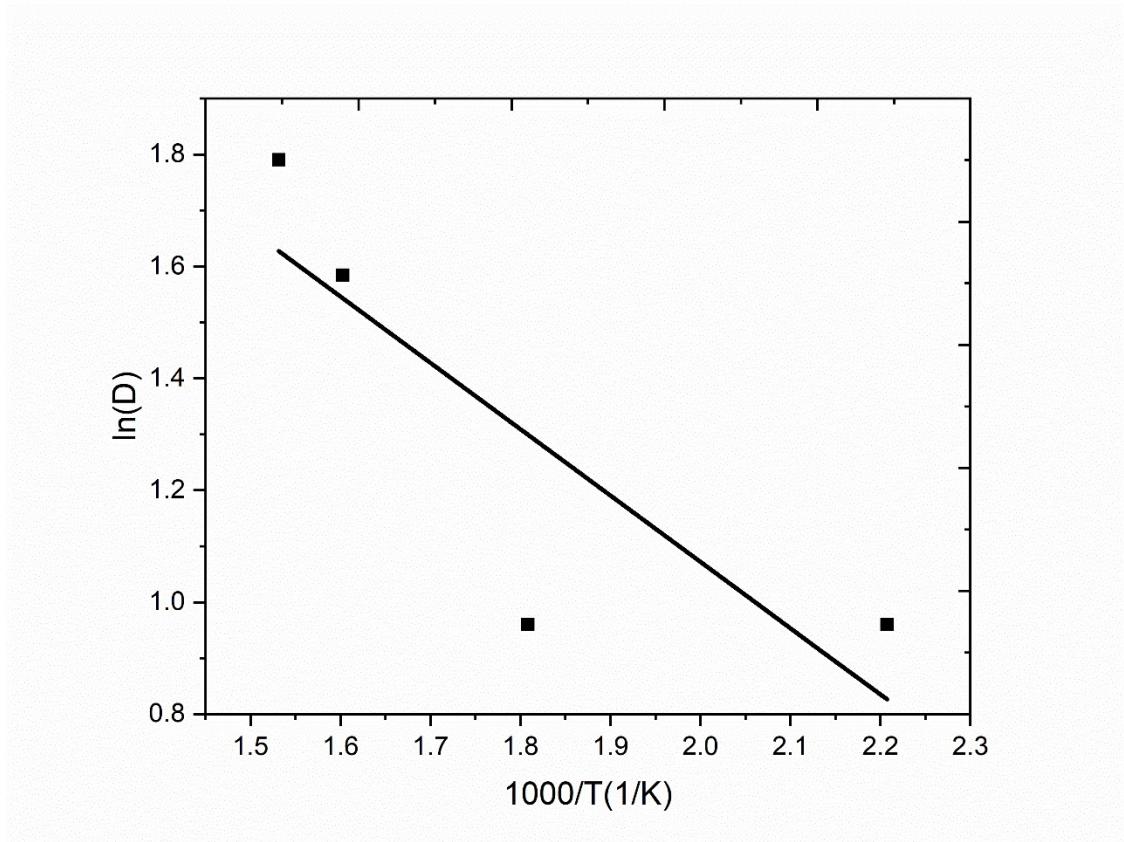


Figure S2. Arrhenius representation of the self-diffusion coefficients of propylene.

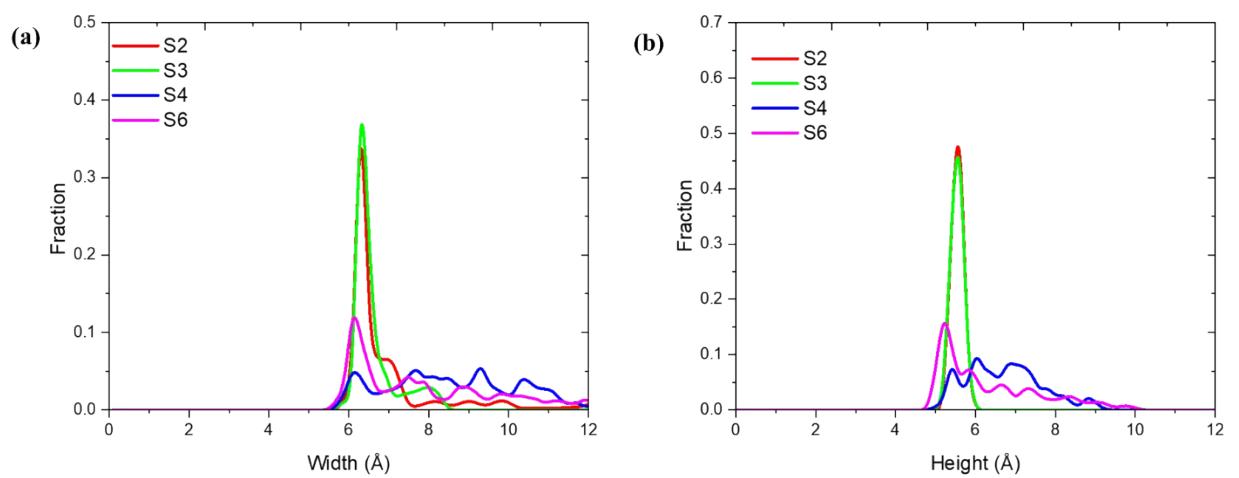


Figure S3. The distribution of (a) height (b) width for propylene molecule inside MFI zeolite at different temperatures

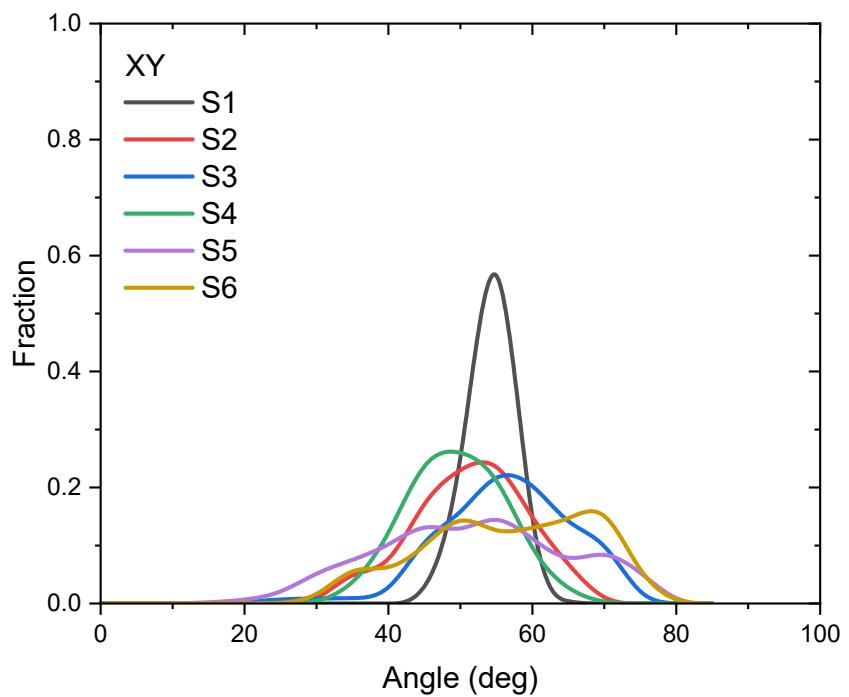
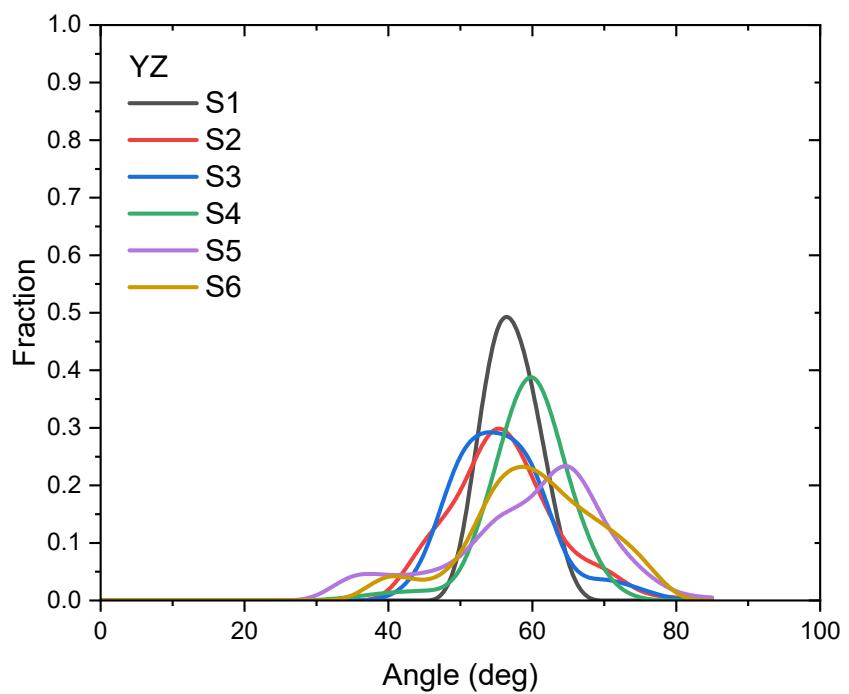


Figure S4. Angle distribution of propylene molecules with respect to the xz plane.

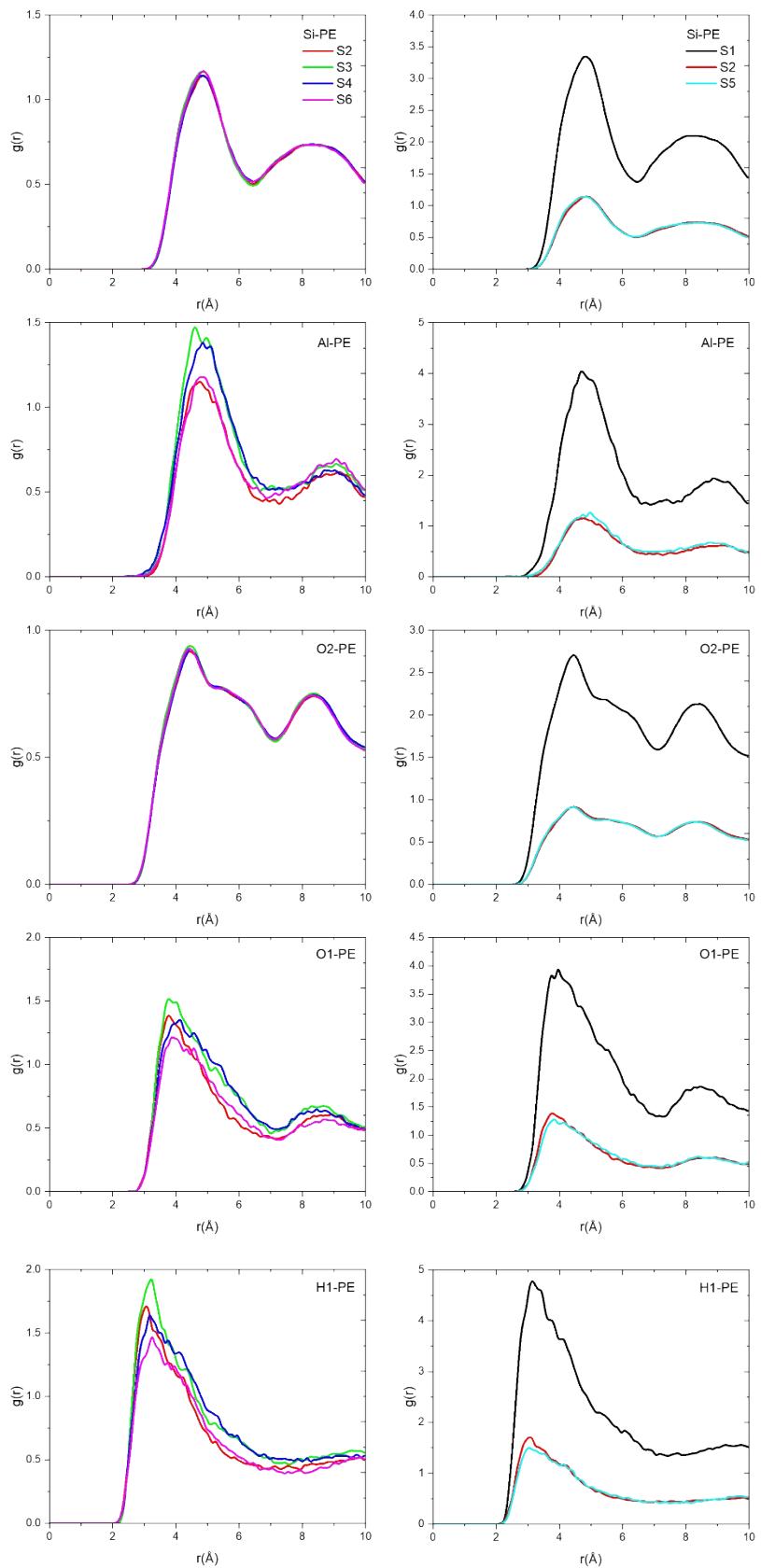


Figure S5. Radial distribution function of propylene molecules and each atom in MFI for all systems at different temperatur