Multiscale Simulation on Product Distribution from Pyrolysis of Styrene–Butadiene Rubber

Shengwei Deng^{1*}, Han Zhuo¹, Yinbin Wang¹, Shuai Leng^{2*}, Guilin Zhuang¹, Xing Zhong¹, Zhongzhe Wei¹, Zihao Yao¹ and Jian-guo Wang^{1*}

¹ Institute of Industrial Catalysis, College of Chemical Engineering, State Key Laboratory Breeding Base of Green-Chemical Synthesis Technology, Zhejiang University of Technology, Hangzhou 310014, P. R. China.

²Qingdao Ecostar Intelligent Equipment Co., Ltd, Qingdao 266400, P. R. China.



Fig. S1 Time evolution of pyrolysis product distributions of homopolymers at 3000 K, (a) polystyrene, (b) 1,2-

polybutadiene, (c) cis-1,4-polybutadiene and (d) trans-1,4-polybutadiene.



Fig. S2 Time evolution of pyrolysis product distributions of multiblock copolymers at 1500 K, (a) A and B-based segments, (b) A and C-based segments, (c) A and D-based segments, (d) B and C-based segments, (e) B and D-based segments and (f) C and D-based segments.



segments, (b) A and C-based segments, (c) A and D-based segments, (d) B and C-based segments, (e) B and D-based segments and (f) C and D-based segments.



segments, (b) A and C-based segments, (c) A and D-based segments, (d) B and C-based segments, (e) B and D-based segments and (f) C and D-based segments.



Fig. S5 Time evolution of pyrolysis product distributions of multiblock copolymers at 3000 K, (a) A and B-based segments, (b) A and C-based segments, (c) A and D-based segments, (d) B and C-based segments, (e) B and D-based segments and (f) C and D-based segments.



Fig. S6 Time evolution of the total number of pyrolysis products of homopolymers at different temperatures.