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RP-3 高温氧化初始阶段反应机理的 ReaxFF MD 模拟

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Initial Reaction Mechanism of RP-3 High Temperature Oxidation Simulated with ReaxFF MD

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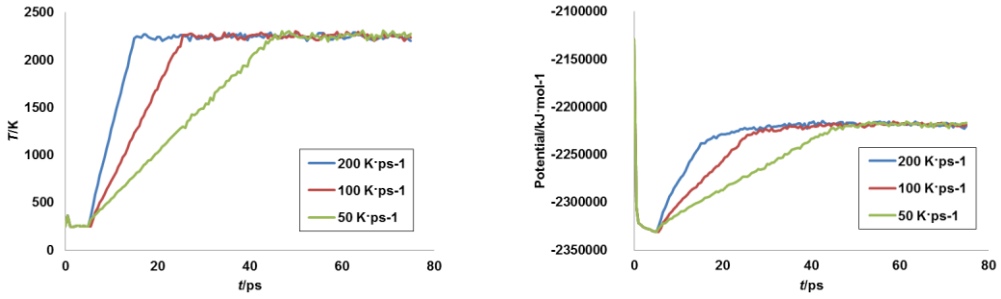

(a) (b)

图 S1　不同升温速率对 ReaxFF MD 模拟的 RP-3 高温氧化体系初始反应状态的影响

Fig.S1　Effects of different heating rate on the initial state in the RP-3 high temperature oxidation simulations by ReaxFF MD

(a) temperature; (b) potential

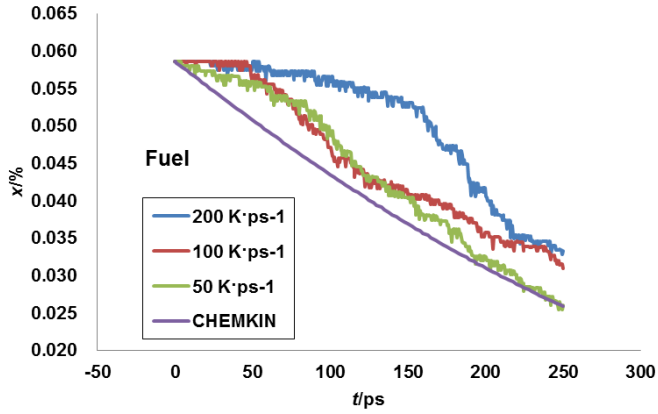

图 S2　初始模型是否升温对 RP-3 高温氧化体系 ReaxFF MD 的 NVT 模拟的影响

Fig.S2　Effects on the evolution tendency of fuel molecules imposed by heating-up of the initial model in RP-3 high temperature oxidation simulations by ReaxFF MD using NVT ensemble