

# Pyrolysis of binary fuel mixtures at supercritical conditions: a study

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Structural evolutions of small aromatic mixtures under extreme temperature conditions: Insights from ReaxFF molecular dynamics investigations. <i>Carbon</i> , 2019, 155, 309-319.	10.3	10
2	Multiply accelerated ReaxFF molecular dynamics: coupling parallel replica dynamics with collective variable hyper dynamics. <i>Molecular Simulation</i> , 2019, 45, 1265-1272.	2.0	11
3	Multi-scale modeling of gas-phase reactions in metal-organic chemical vapor deposition growth of WSe <sub>2</sub> . <i>Journal of Crystal Growth</i> , 2019, 527, 125247.	1.5	59
4	Reaction Mechanisms in Pyrolysis of Hardwood, Softwood, and Kraft Lignin Revealed by ReaxFF MD Simulations. <i>Energy &amp; Fuels</i> , 2019, 33, 11210-11225.	5.1	36
5	ReaxFF molecular dynamics study on the pyrolysis process of cyclohexanone. <i>Journal of Analytical and Applied Pyrolysis</i> , 2019, 141, 104620.	5.5	41
6	Atomistic Scale Analysis of the Carbonization Process for C/H/O/N-Based Polymers with the ReaxFF Reactive Force Field. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5357-5367.	2.6	123
7	Diagnosing the Impact of External Electric Fields Chemical Kinetics: Application to Toluene Oxidation and Pyrolysis. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3080-3089.	2.5	14
8	Thermal Hydrogenation and Degradation of Quinoline from Reactive Force Field Simulations. <i>ChemistrySelect</i> , 2019, 4, 12996-13005.	1.5	4
9	Multiscale Simulation on Product Distribution from Pyrolysis of Styrene-Butadiene Rubber. <i>Polymers</i> , 2019, 11, 1967.	4.5	13
10	Pyrolysis mechanism of HFO-1234yf with R32 by ReaxFF MD and DFT method. <i>International Journal of Refrigeration</i> , 2020, 109, 82-91.	3.4	33
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13	Numerical simulations of yield-based sooting tendencies of aromatic fuels using ReaxFF molecular dynamics. <i>Fuel</i> , 2020, 262, 116545.	6.4	37
14	Predicting cost-effective carbon fiber precursors: Unraveling the functionalities of oxygen and nitrogen-containing groups during carbonization from ReaxFF simulations. <i>Carbon</i> , 2020, 159, 25-36.	10.3	59
15	ReaxFF-based molecular dynamics study of bio-derived polycyclic alkanes as potential alternative jet fuels. <i>Fuel</i> , 2020, 279, 118548.	6.4	35
16	ReaxFF Reactive Molecular Dynamics Simulations of Mechano-Chemical Decomposition of Perfluoropolyether Lubricants in Heat-Assisted Magnetic Recording. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22496-22505.	3.1	17
17	Molecular dynamics simulation of soot formation during diesel combustion with oxygenated fuel addition. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20829-20836.	2.8	23
18	Reactive Molecular Dynamics Simulations and Quantum Chemistry Calculations To Investigate Soot-Relevant Reaction Pathways for Hexylamine Isomers. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4290-4304.	2.5	11

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