

Correction to Adaptive Accelerated ReaxFF Reactive Dynamics with Validation from Simulating Hydrogen Combustion

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S Supporting Information

The Supporting Information did not include the revised COH ReaxFF force field used for obtaining the published results. The new Supporting Information includes the new parameters on pages 16–19.

■ ASSOCIATED CONTENT

S Supporting Information

H₂O generation curves of all 19 samples, H₂O generation curves of $\Delta V^{\max} = 50, 60, 70$ and 80, potential energy and force curves, H₂ loss curve at 2498 K, H₂O₂ generation curve at 2498 K, species generated in aARRDYN simulations with $\Delta V^{\max} = 20$ and 40 kcal at 2498 K; the new ReaxFF–OH2014 force field parameters plus some of the validations against QM; results for the Arrhenius analysis, reaction mechanisms and kinetics from the older ReaxFF–CHO2008 force field, the force field file, and the plot script. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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