

Supplementary Materials: Reactive Molecular Dynamics Study of the Thermal Decomposition of Phenolic Resins

Marcus Purse, Grace Edmund, Stephen Hall, Brendan Howlin, Ian Hamerton and Stephen Till

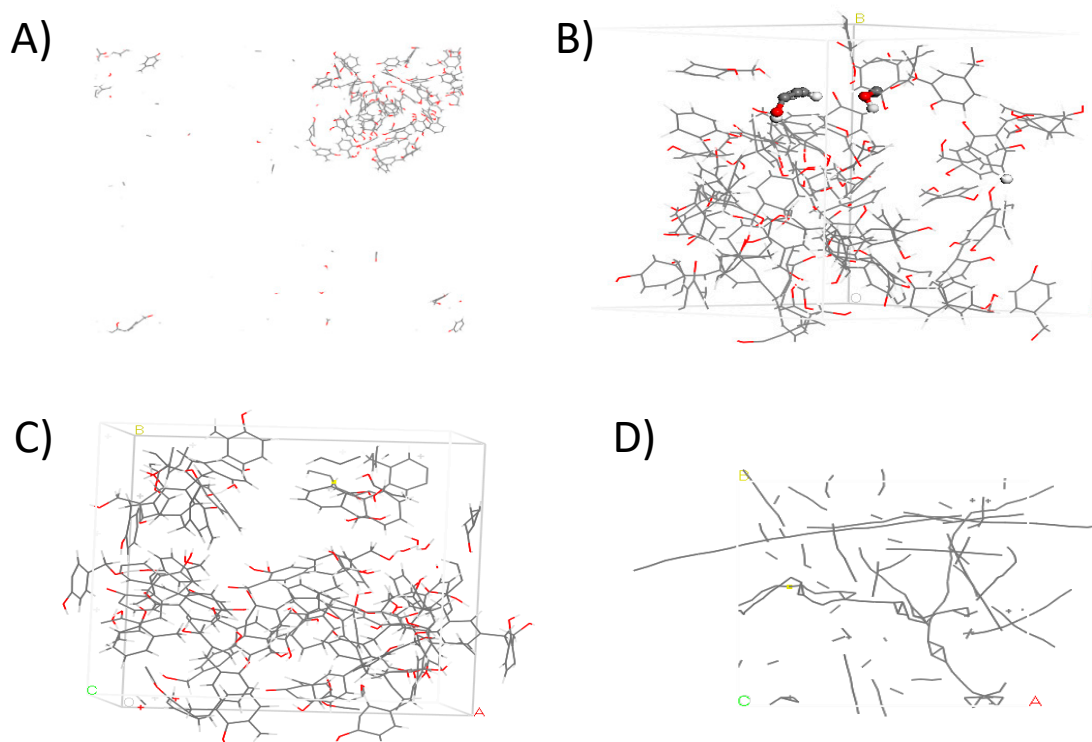


Figure S1. (A) Model of 1000 atoms, 33% cured at 1250 K after 5 ps. (B) close up of (A), showing broken chains, (C) Model of 1000 atoms, 66% cured at 1250 K after 10 ps. (D) Model of 1000 atoms, 66% cured at 1250 K after 1.5 ns, showing cyclopropane rings.