Electronic Supplementary Material (ESI) for RSC Mechanochemistry.

Atomistic simulations of mechanically activated reactions for oxygen release from polymers

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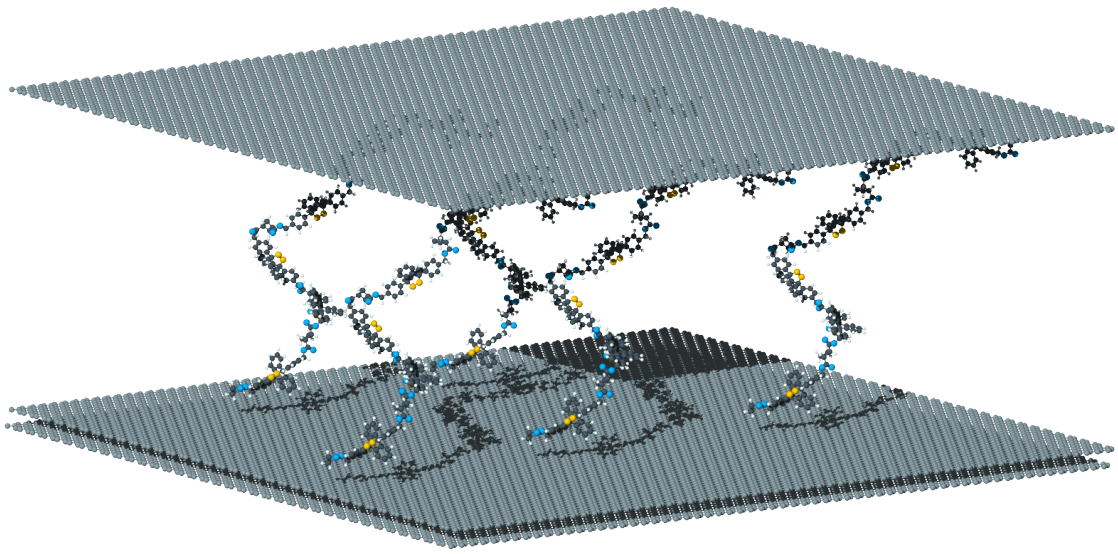

Figure S1: Snapshot of the simulation box for the shear-driven reactions, before compression and sliding. The white and black spheres represent hydrogen and carbon atoms, respectively. The grey spheres represent carbon atoms from the graphite slabs. The blue and gold spheres represent oxygen atoms, where the gold color is used to identify the atoms that will be released as oxygen singlets.

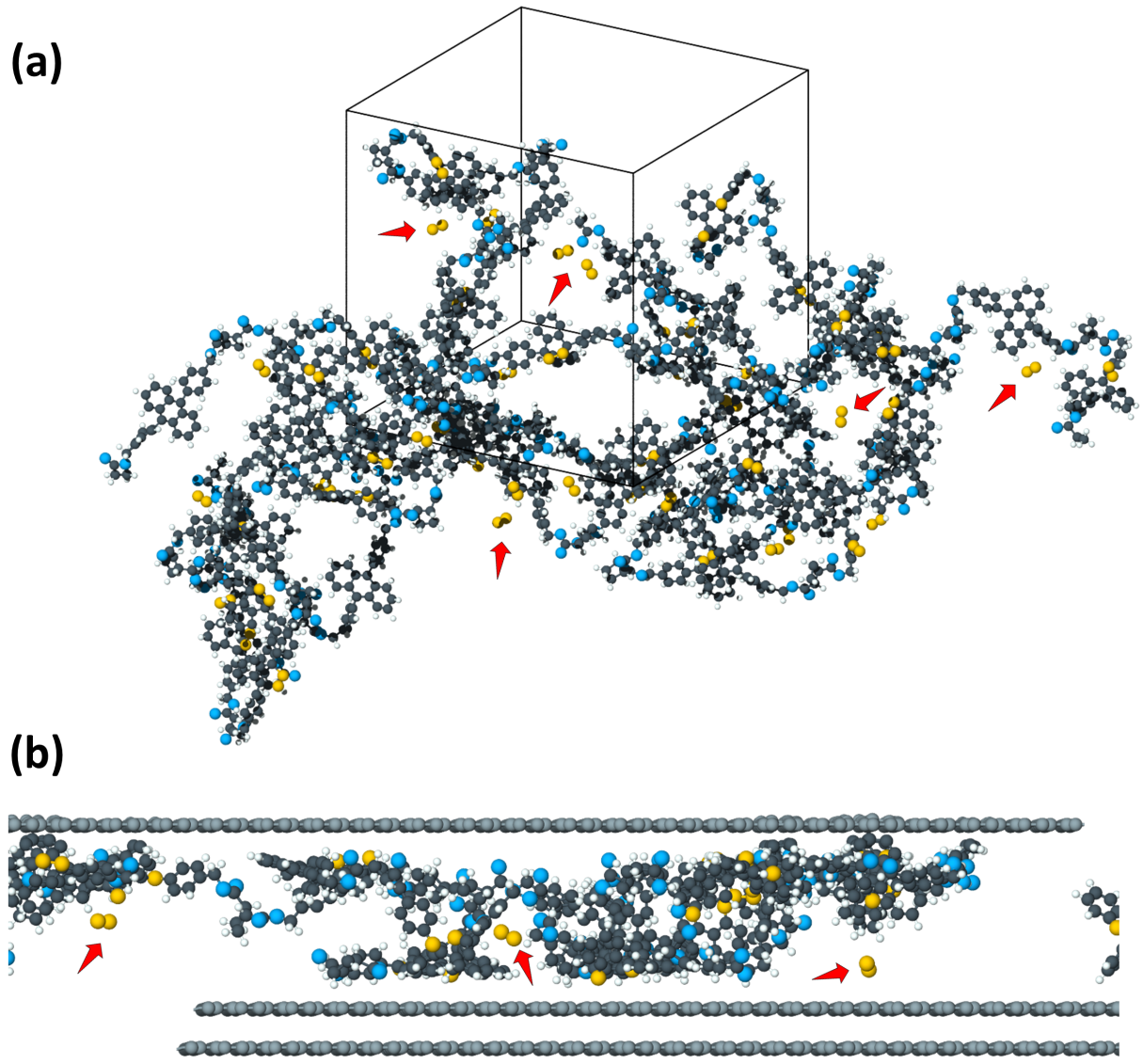

Figure S2: Free oxygen molecules released from the anthracene groups in a (a) heating simulation and (b) shearing simulation. The free oxygen molecules are identified by red arrows. The atom color scheme is the same as in Fig. S1.

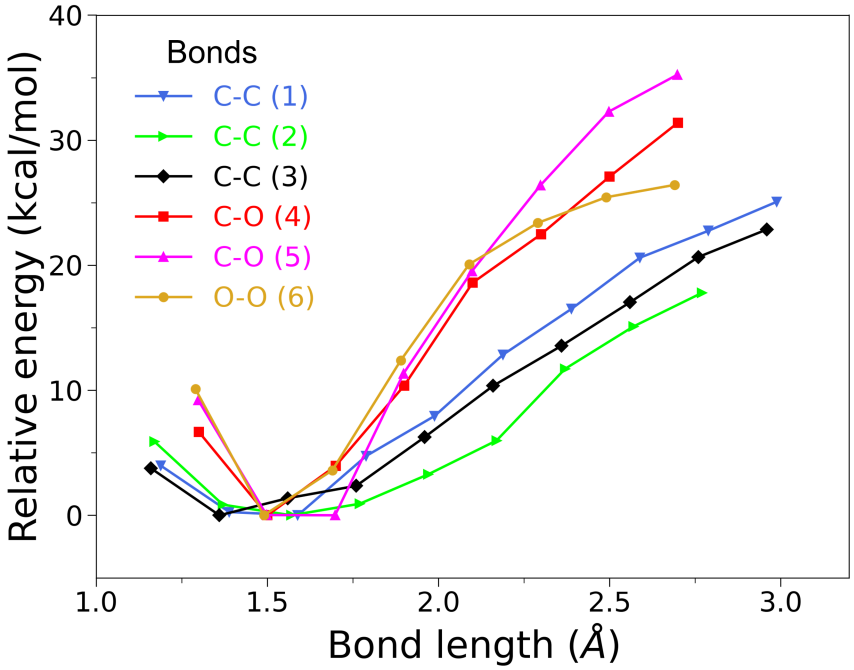

Figure S3: Relative energy as a function of bond length from the DFT-based relaxed coordinate scans. The PMA-EPO monomer was built using Schrödinger Maestro v. 2022-3.[?] The monomer and the bonds included in the relaxed coordinate scan are shown in Fig. 1a. The peroxide group is bonded to the middle ring of the anthracene group of the monomer. The relaxed scan was conducted using Jaguar at the M06-2X/6-311+G* level of theory. For each bond, the relaxed scan consisted of geometry optimizations at fixed lengths in step sizes of 0.2 Å. The maximum number of iterations was set to the default value of 100. For bond lengths around 1.8 to 3 Å, the lengths at which such bonds dissociate, the highest relative energy is observed for the C–O bond 5.

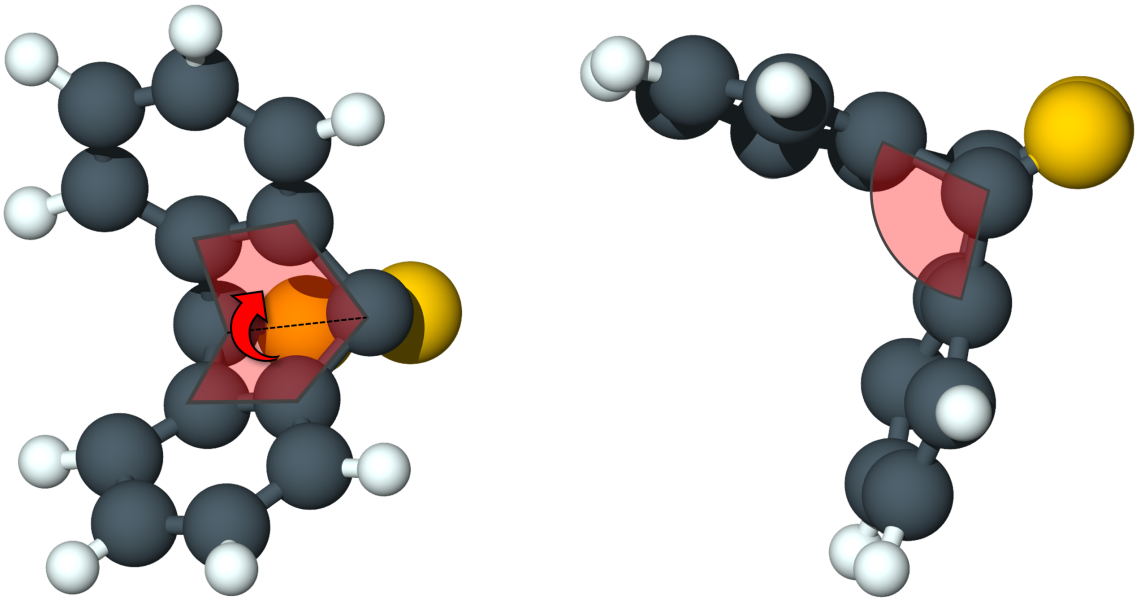

Figure S4: Snapshot of the anthracene ring showing the central anthracene angle used for the deformation analysis in Fig. 5. The atom color scheme is the same as in Fig. S1.