

Studies of the Mechanically Induced Reactivity of Graphene with Water Using a 2D-Materials Strain Reactor

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Supplementary Information

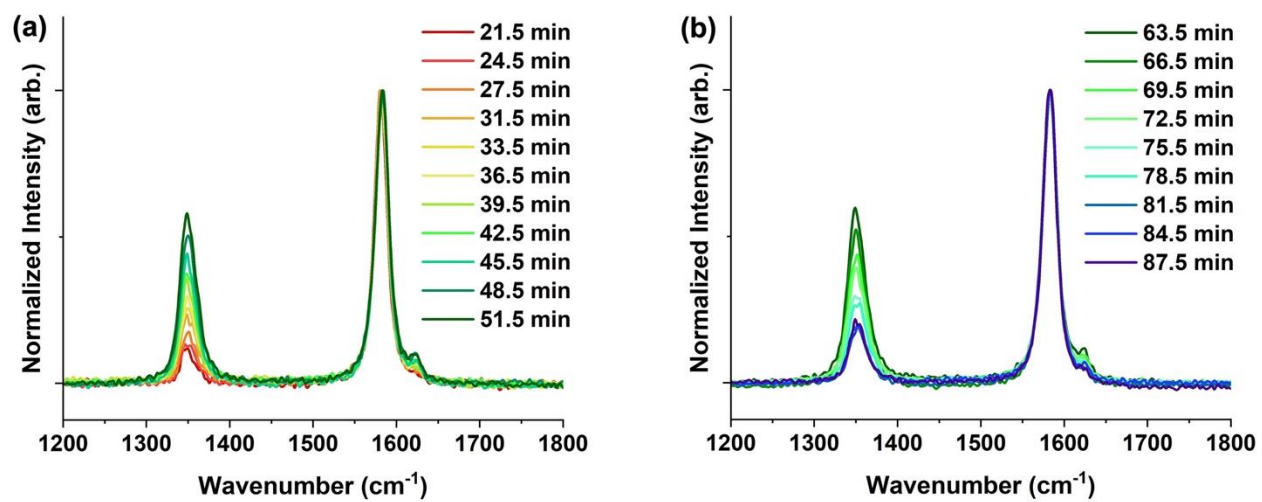
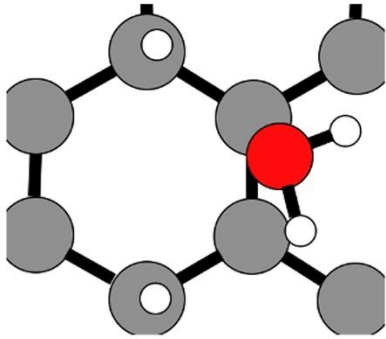
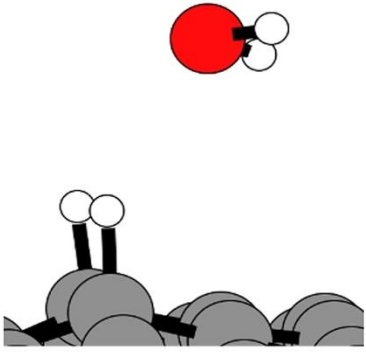
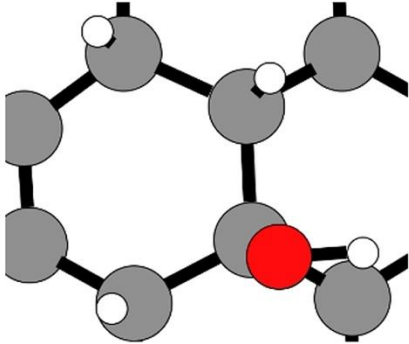
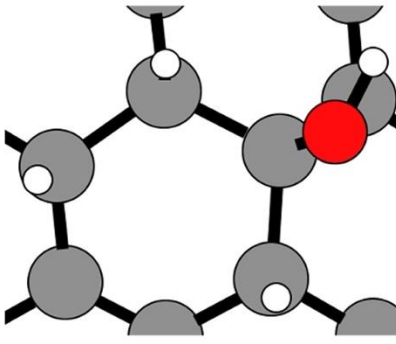


Figure S1. Full set of time-resolved spectra for reaction of graphene with pressurized water as referenced in the main text (Figure 5).

Table S1. Water Dissociation with H* on Flat & Curved Graphene.

	Flat	Curved
Initial State		
Final State		
ΔE (eV)	1.91	1.66

Two H* defects are considered at the same time for maintaining a neutral graphene surface. With two H* defects introduced, Table S1 includes the configurations of initial and final states of water dissociation on flat/curved graphene. The energy difference between final state and initial state shows that curvature makes dissociated water adsorption more favorable. Red = O, gray = C, white = H.

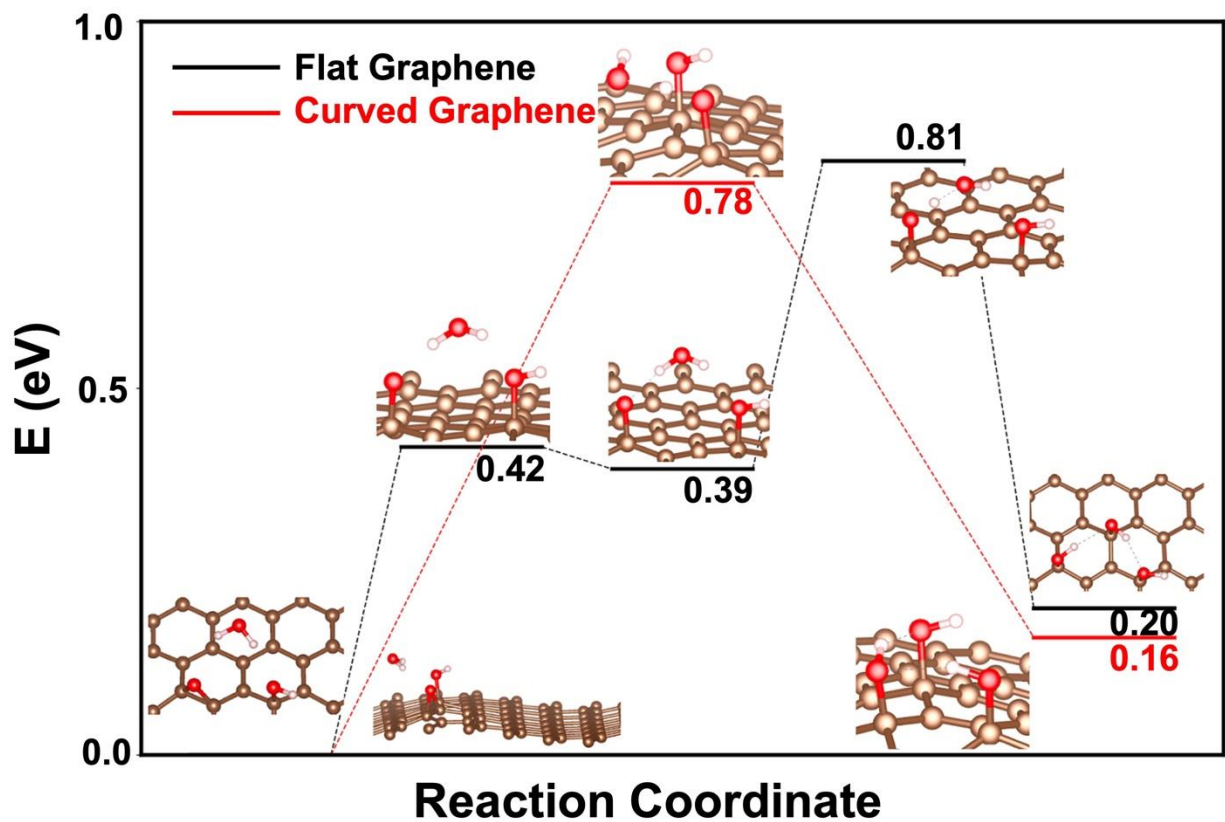


Figure S2. Water dissociation with OH*/O on flat and curved graphene. OH* also helps water dissociation by decreasing the activation barrier.

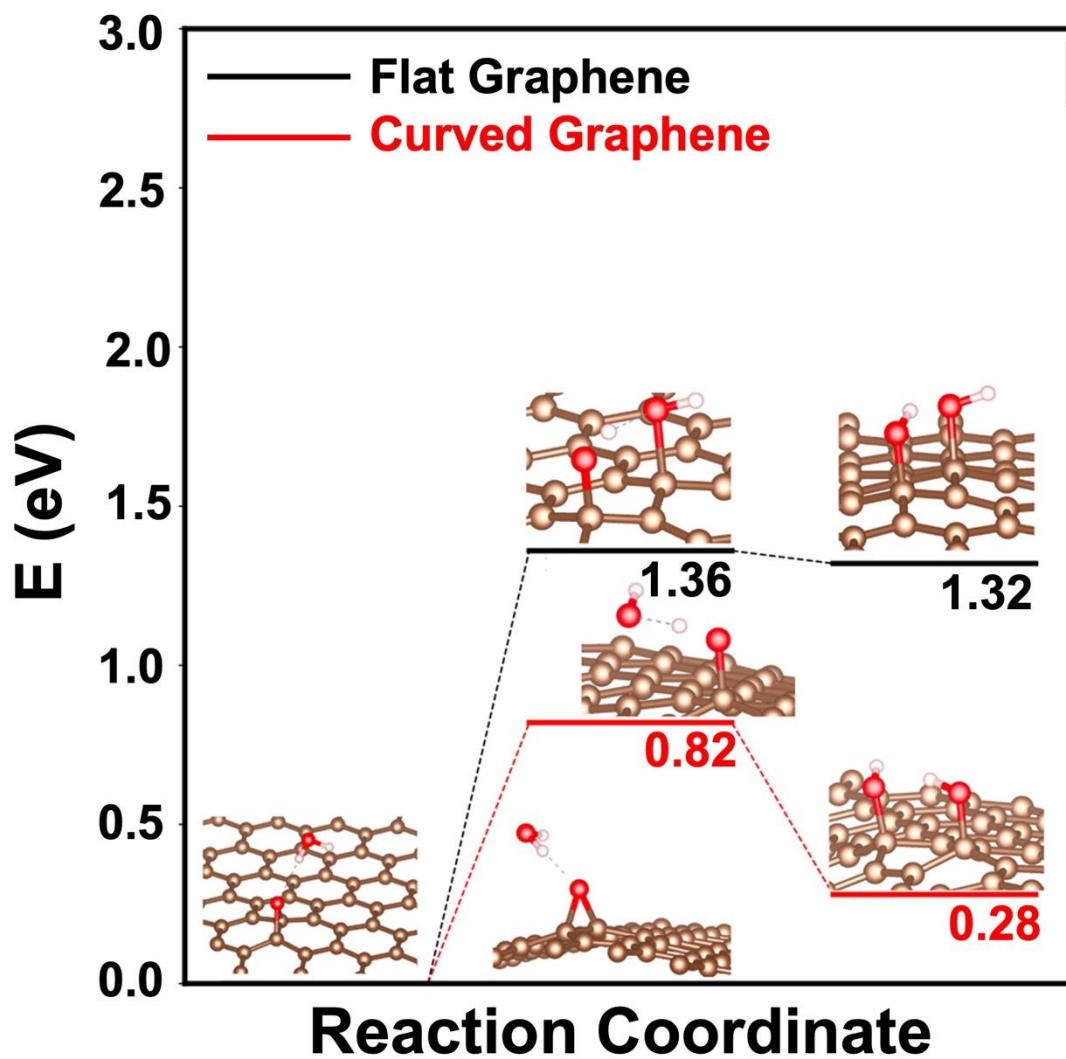


Figure S3. Water dissociation with one epoxide defect on flat and curved graphene.

Data Availability Statement

Raw data files for results presented herein, in addition to high resolution copies of the figures in both the main text and supplementary information, can be accessed at the link below:

<https://doi.org/10.6084/m9.figshare.26765020>.