Supporting Information

Selective Tuning of a Particular Chemical Reaction on Surfaces Through Electrical Resonance: an *ab Initio* Molecular Dynamics Study

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Phonon spectrum was calculated using density functional perturbation theory, as implemented in Quantum Espresso Phonon package. The considered system of OH adsorbed graphene system is shown in the inset of Figure S1(a). The total phonon density of states (PhDOS) is shown in Figure S1(a). Figure S1(b) shows the partial PhDOS projected onto O atom: the weight for O atom in each phonon eigenvector is multiplied when we add up the phonon density of states. It is noticeable that the PhDOS has peak near 0.024 fs^{-1}, as indicated by the upward arrow. This value is in close agreement with the RF 0.025 fs^{-1} calculated from the fast Fourier transform (FFT) analysis for the time series *Z(t)* shown in Figure 2(b) and 2(c) of the main text.

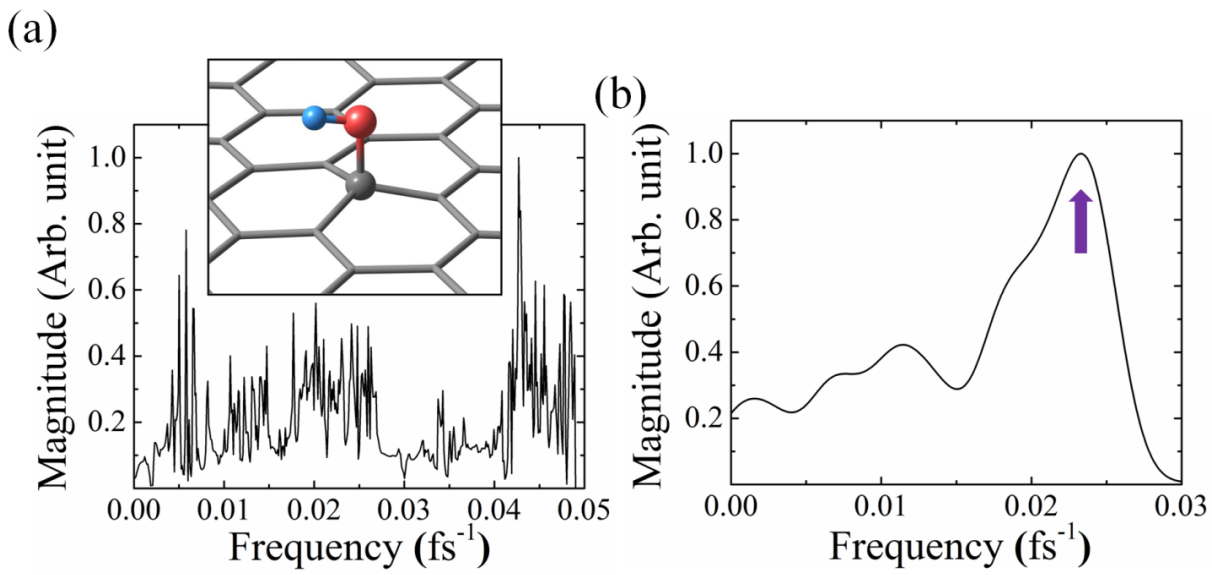

Figure S1. (a) The total phonon density of states of the OH adsorbed graphene system. (b) The total phonon density of states projected onto the vibration of O atom. Inset is a zoomed-in view of the equilibrium geometry.

We consider the replacement of an epoxy functional group on the graphene with NH_2. In the initial state (IS) configuration, NH_3 is present near the epoxy oxygen of GO, as shown in Figure S2(a). The final state (FS) aminated configuration is presented in Figure S2(c). We first searched for the TS from the IS to the FS, as depicted in Figure S2(c). In the TS, shown as the inset of Figure S2(b), one of the C–O bonds is broken and, at the same time, one of the hydrogen atoms of the NH_3 is moved towards the oxygen, and its remainder appears as NH_2 on the surface. The NEB calculated ΔE value of 0.78 eV along with the MEP is shown in Figure S2(b).

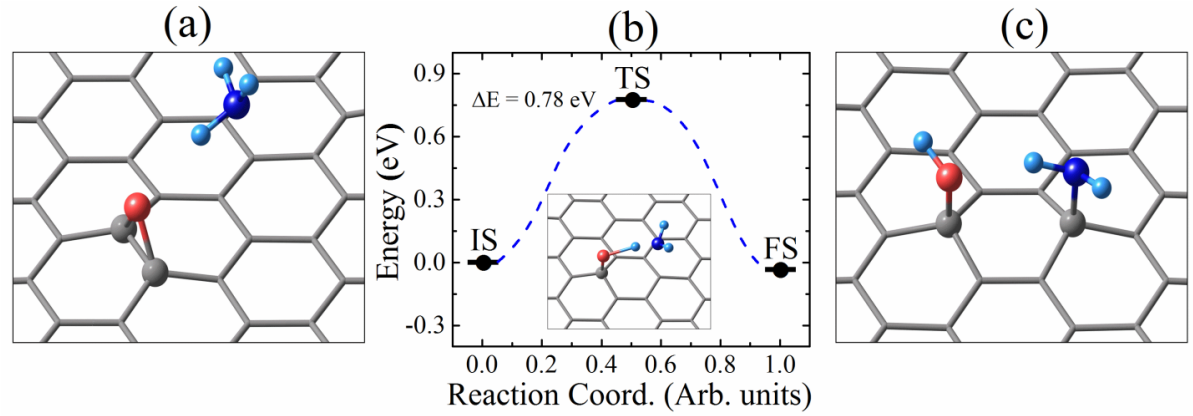

Figure S2. Initial, transition and final state configurations for the amination process of the graphene from an epoxy functional group on graphene are represented by (a), the inset of (b) and (c), respectively.