Supplementary material for "Laser-pulse induced water decomposition above two-dimensional materials as seen via time-dependent density functional theory "

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The decomposition of an isolated H_2O molecule by a femtosecond laser was simulated. The results with time-dependent density functional theory (TDDFT) using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional are shown in Fig. S.1. Computational conditions were the same as those using the local density approximation (LDA) described in the main text. The starting geometry was determined by the geometry optimization using the PBE functional.

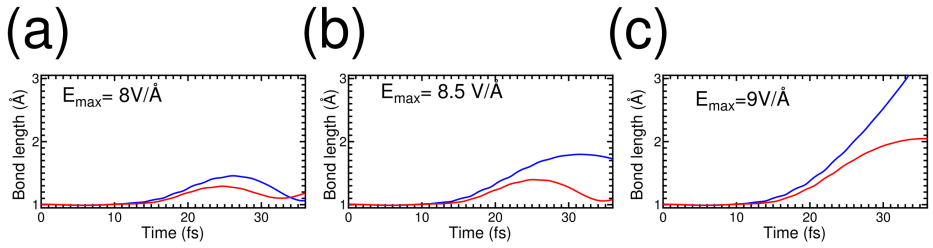

FIG. S.1: (Color online) Time evolution of the O-H bond length of an isolated H_2O molecule under a pulsed laser with a full width at half-maximum of 10 fs and a wavelength of 800 nm. The assumed maximum intensity of laser field is (a) 8 V/Å, (b) 8.5 V/Å, and (c) 9 V.Å. With E_{max}=9V/Å, one of the two O-H bonds (blue curve) was broken.

The decomposition of an H_2O molecule above a graphene sheet calculated with TDDFT using GGA with the PBE functional is shown in Fig. S.2. Computational conditions were the same as those using the LDA described in the main text. The starting geometry was determined by the geometry optimization using the PBE functional, which gave a slightly longer distance between the H_2O molecule and the graphene sheet than that obtained by the LDA.

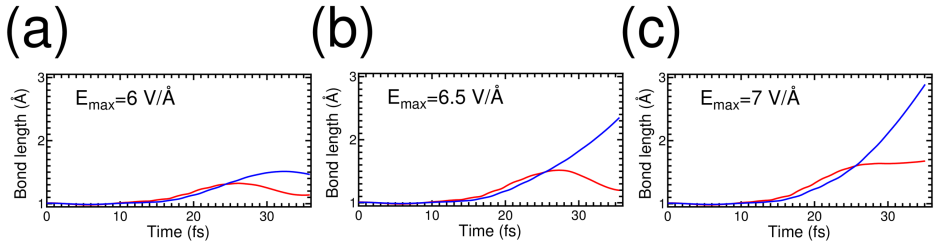

FIG. S.2: (Color online) Time evolution of O-H bond length of an H_2O molecule above a graphene sheet under a pulsed laser with a full width at half-maximum of 10 fs and a wavelength of 800 nm. The assumed maximum intensity of laser field is (a) 6 V/Å, (b) 6.5 V/Å, and (c) 7 V.Å. With E_{max}=6.5 V/Å and 7 V/Å, one of the two O-H bonds (blue curve) was broken.

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