Supplementary Materials for

Adsorption and Reaction Mechanism of Single and Double H_2O Molecules on Graphene Surface with Defects: A Density Functional Theory Study

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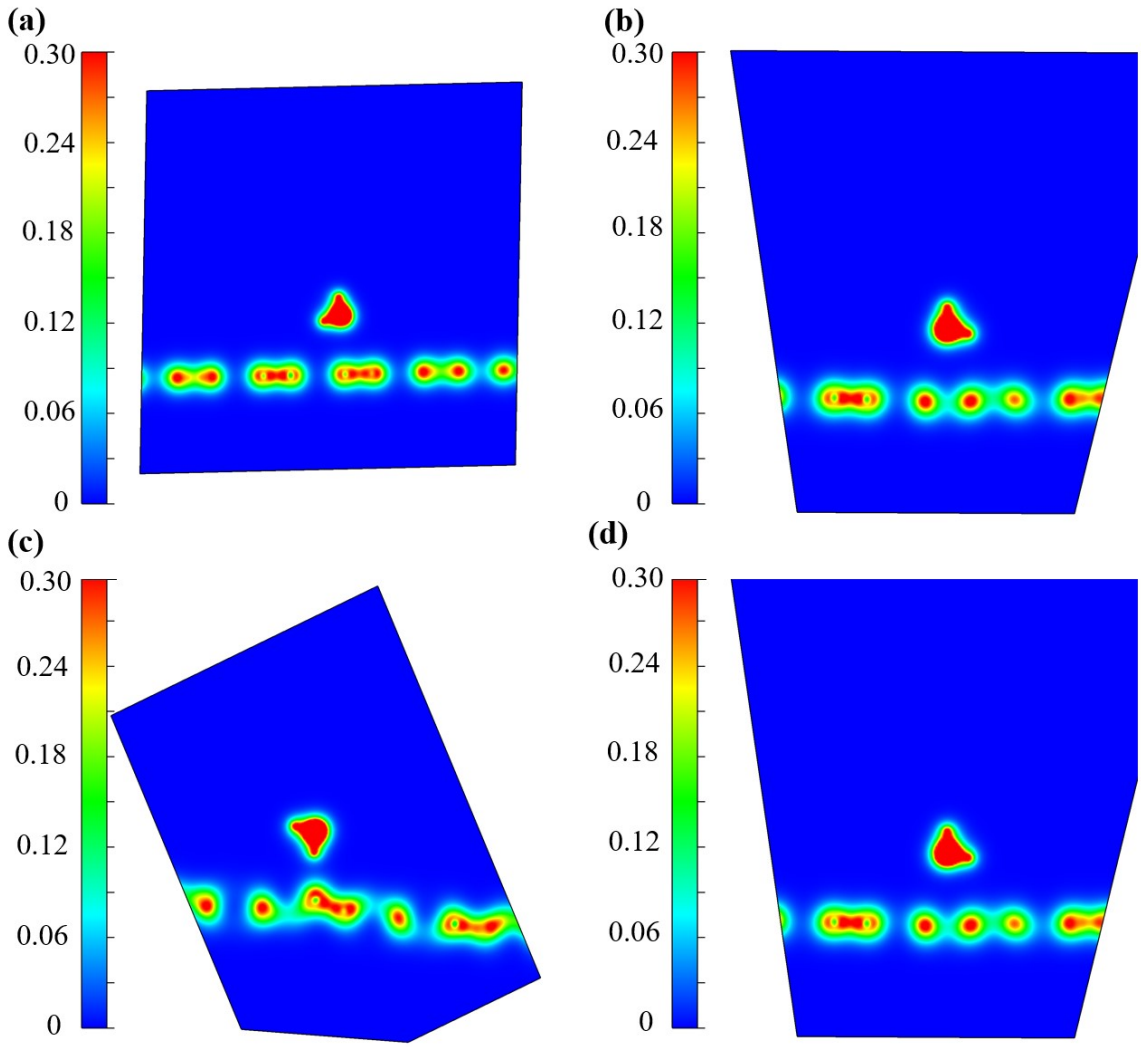

Fig. S1. The charge density of the optimal physical adsorption configuration (Fig.1. in the paper) **on the four surfaces: (a) pristine graphene surface; (b) SW defect surface; (c) single vacancy defect surface; (d) double vacancy defect surface;** (take the three atoms of the water molecule as a plane to cut the plane)

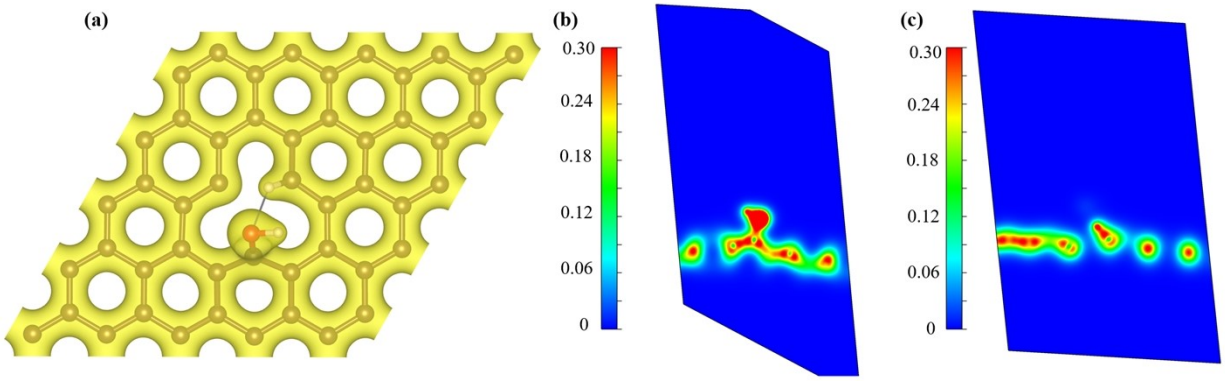

Fig. S2. The charge density distribution of 1C configuration (fig.6. in the paper) (a) in 3D; (b) on the plane of the hydroxyl group; (c) on the plane of the C-H bond

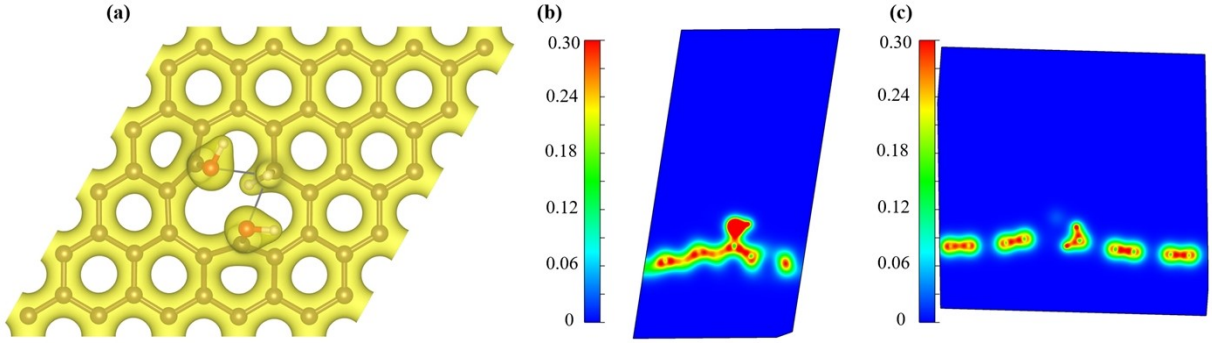

Fig. S3. The charge density distribution of 2C configuration (fig.7. in the paper) (a) in 3D; (b) on the plane of the hydroxyl group; (c) on the plane of the C-H bond

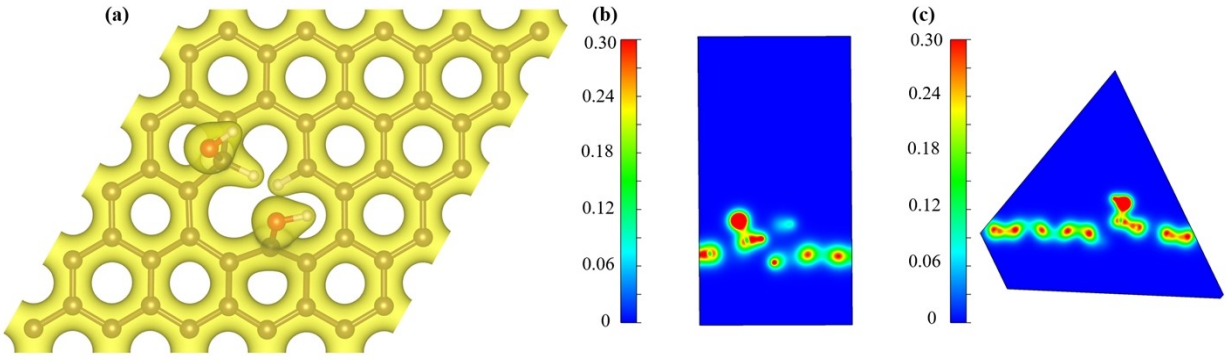

Fig. S4. The charge density distribution of 2E configuration (fig.7. in the paper) (a) in 3D; (b) on the plane of the hydroxyl group; (c) on the plane of the C-H bond

Table S1. Comparison of the calculation results of different vdw corrections. (For the top site of the PG surface)

PG top	u	d	p	vd	vu
vdW-DF2	-0.11191	-0.11506	-0.11479	-0.12288	-0.12915
vdW-DF	-0.13418	-0.13372	-0.13115	-0.13444	-0.14748
DFT-D2	-0.08034	-0.12442	-0.12464	-0.13268	-0.13037
DFT-D3	-0.08797	-0.12361	-0.12328	-0.12832	-0.12918

Table S2. Charge transfer of the four optimal physical adsorption configurations (C1 represents the carbon atom that interacts with the OH bond of H_2O molecule, C2, C3, and C4 are the three carbon atoms closest to C1 respectively)

	PG	SW	SV	DV
C1	0.014	0.0097	0.0421	0.0203
C2	0.0067	0.0092	-0.0013	0.0071
C3	0.0068	-0.0061	-0.0021	0.0044
C4	-0.0029	-0.0003	-0.0019	-0.0023

Table S3. The maximum energy span of the possible paths for the formation of single water molecule adsorption configuration (corresponding to Fig.6 in paper).

Configuration	PATH	Energy barrier
1C	SV-1C	0.55 eV
1A	SV-1C-1A	1.47 eV
1D	1) SV-1C-1A-1D	1.47 eV
	2) SV-1C-1E-1D	1.49 eV
1E	SV-1C-1E	0.55 eV
1F	SV-1C-1A-1F	1.47 eV