

## Supplementary Electronic Information: Platinum Single-atom Adsorption on Graphene: A Density Functional Theory Study

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## I. PRELIMINARY

In this Electronic Supplementary Information, we present functional dependence of the binding energy of the single Pt atom on graphitic materials and the GNR stability, the width dependence of GNRs, density of states projected onto atomic orbitals for  $\text{Pt}_{\text{C}_\alpha} @ z_1$ , which gives the core level shift agreeing with the experiment, Bader charge of the single Pt atom adsorbed on graphene and graphene nanoribbons (GNRs) obtained using the Bader charge analysis code<sup>1-4</sup>.

## II. FUNCTIONAL DEPENDENCE OF THE BINDING ENERGIES OF THE SINGLE PT ATOM ON GRAPHITIC MATERIALS

TABLE S1. Binding energies of the single Pt atom on graphitic materials calculated using the Perdew-Burke-Ernzerhof functional. The unit of energy is eV.

Structure	$E_b$
Pt/GR	-1.61
Pt/V <sub>1</sub>	-7.35
Pt/V <sub>2</sub>	-7.29
Pt/GB-GR	-2.20
Pt/DisGR	-2.69

### III. FUNCTIONAL DEPENDENCE OF THE GRAPHENE NANORIBBON STABILITY

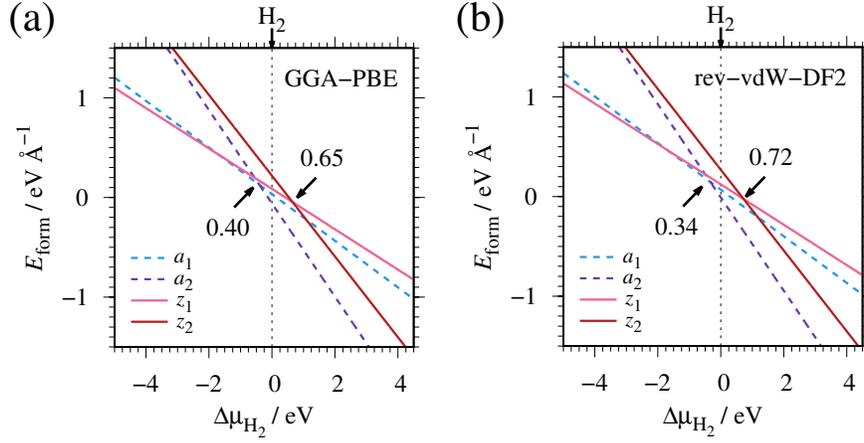


FIG. S1. Formation energies ( $E_{\text{form}}$ ) of armchair and zigzag graphene nanoribbon as a function of chemical potential of hydrogen molecule  $\mu_{\text{H}_2}$ , calculated using (a) PBE and (b) rev-vdW-DF2. 20-*a*GNR and 10-*z*GNR were used.

### IV. WIDTH DEPENDENCE OF THE GRAPHENE NANORIBBON STABILITY

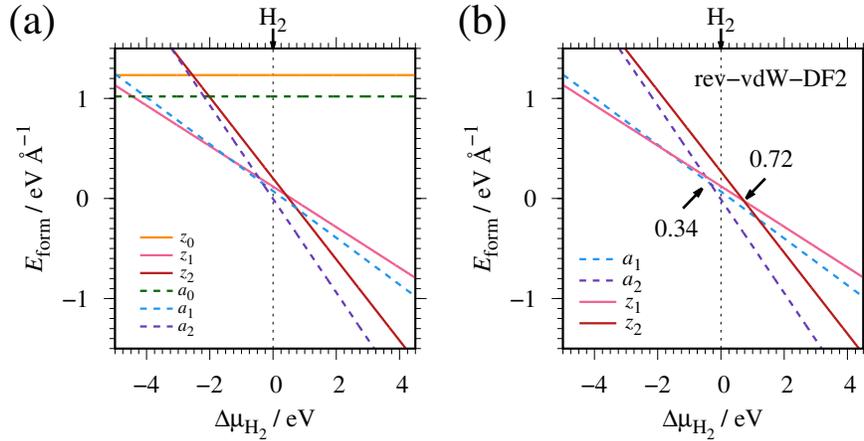


FIG. S2. Formation energies ( $E_{\text{form}}$ ) of armchair and zigzag graphene nanoribbon as a function of chemical potential of hydrogen molecule  $\mu_{\text{H}_2}$ , calculated with (a) 10-*a*GNR and 5-*z*GNR and (b) 20-*a*GNR and 10-*z*GNR.

## V. DENSITY OF STATES

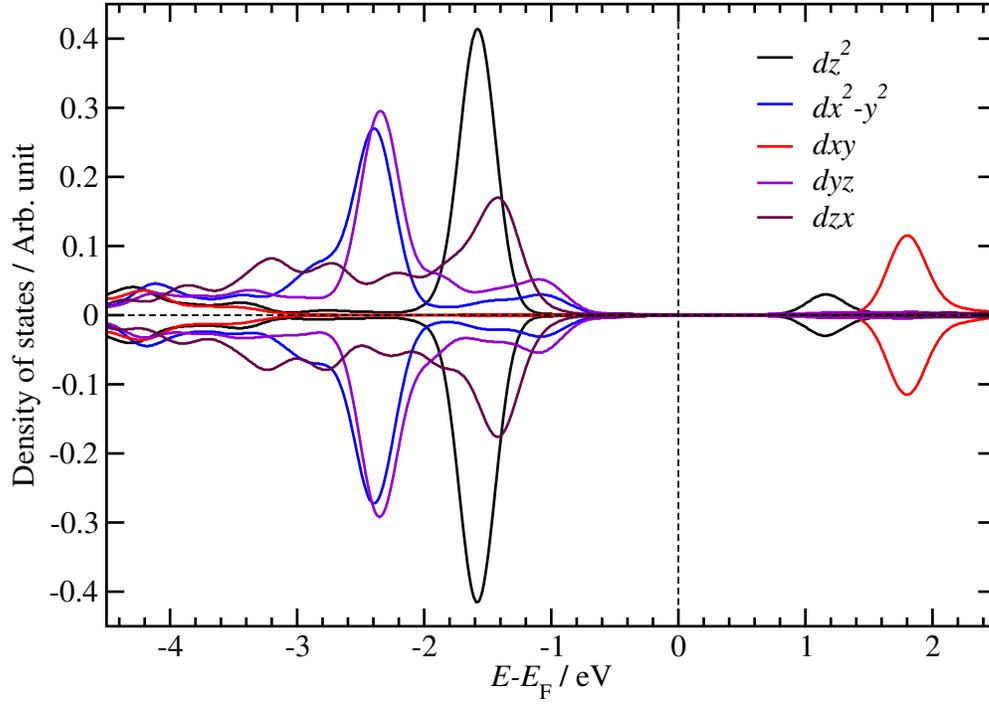


FIG. S3. Densities of states projected onto the Pt  $d$  orbitals for  $\text{Pt}_{C_{\alpha}}@z_1$ . The energy origin is set to the Fermi level ( $E_F$ ).

## VI. BADER CHARGE

TABLE S2. Bader charge ( $Q_{\text{tot}}$ ) of the Pt atom and the deviation from the charge of the isolated atom ( $\Delta Q_{\text{tot}}$ ) along with the calculated core level shift (CLS).

Structure	$Q_{\text{tot}}$	$\Delta Q$	CLS
Pt/GR	9.94	-0.06	
Pt/V <sub>1</sub>	9.51	-0.49	
Pt/V <sub>2</sub>	9.24	-0.76	
Pt <sub>T</sub> @z <sub>0</sub>	9.80	-0.20	-0.56
Pt <sub>B</sub> @z <sub>0</sub>	9.69	-0.31	0.44
Pt <sub>C<sub>α</sub></sub> @z <sub>0</sub>	9.62	-0.38	0.50
Pt <sub>C<sub>β</sub></sub> @z <sub>0</sub>	9.36	-0.54	1.44
Pt <sub>C<sub>β</sub>C<sub>γ</sub></sub> @z <sub>0</sub>	9.23	-0.77	1.67
Pt <sub>T</sub> @z <sub>1</sub>	10.11	0.11	-0.93
Pt <sub>C<sub>α</sub></sub> @z <sub>1</sub>	9.72	-0.28	1.43
Pt <sub>C<sub>α</sub>C<sub>β</sub></sub> @z <sub>1</sub>	9.45	-0.55	0.81
Pt <sub>T</sub> @z <sub>2</sub>	10.17	0.17	0.35
Pt <sub>C<sub>β</sub></sub> @z <sub>2</sub>	9.59	-0.31	1.42
Pt <sub>C<sub>β</sub>C<sub>γ</sub></sub> @z <sub>2</sub>	9.56	-0.34	1.11
Pt <sub>LB</sub> @a <sub>1</sub>	9.75	-0.25	0.44
Pt <sub>(C<sub>α</sub>)<sup>2</sup></sub> @a <sub>1</sub>	9.76	-0.24	0.17
Pt <sub>C<sub>α</sub></sub> @a <sub>2</sub>	9.74	-0.26	1.33
Pt <sub>(C<sub>α</sub>)<sup>2</sup></sub> @a <sub>2</sub>	9.78	-0.12	0.51

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