Electronic Supplementary Material for PCCP

Supporting Information

The Use of Nanometer-sized Hydrographene Species for Support Material for Fuel Cell Electrode Catalysts: A Theoretical Proposal

Takashi Yumura[†, *] Keisuke Kimura[†], Hisayoshi Kobayashi[†], Ryo Tanaka[‡], Norio Okumura[‡], and Tokio Yamabe[‡]

Fig. S1 Band structures of graphene obtained by extend Hückel calculation (a) and a more reliable calculated based on density functional theory (PW91).

Fig. S2 Optimized geometries for Pt_6 and Pt_5 clusters.

Fig. S3 Four optimized structures of Pt_5 clusters on $C_{96}H_{26}$ at the B3LYP level of theory. CE represents the center of $C_{96}H_{26}$, and OC represents an obtuse-angled corner. We can distinguish the four structures by Pt_5 cluster shapes as well as whether a Pt_5 cluster binds into an edge or the center of $C_{96}H_{26}$. The number of adsorbed Pt atoms (NAPt) can be also seen.

Table S1 Key geometrical parameters of a Pt_5 cluster on $C_{96}H_{26}$ and their energtics (kcal/mol).

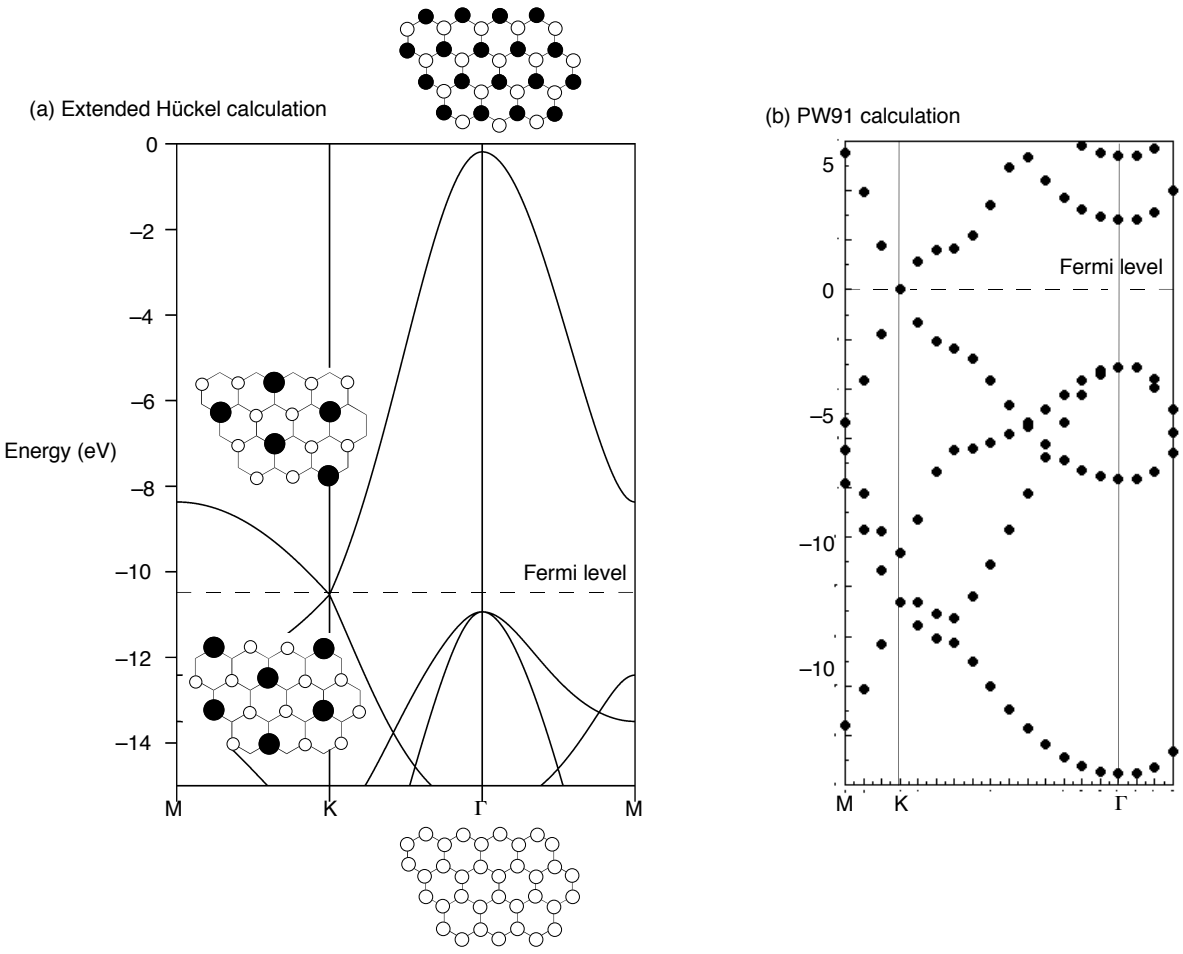
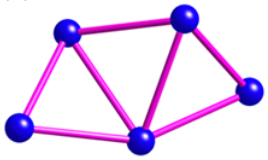


Fig. S1 Band structures of graphene obtained by extended Hückel calcuation (a) and a more reliable calculation based on density functional theory (PW91).

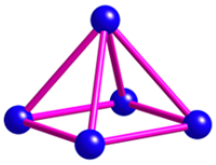
Pt_5

(1)



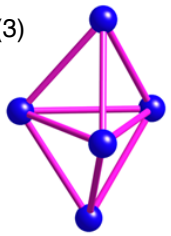
Relative energy
0 kcal/mol
HOMO: –5.67 eV
LUMO: –4.31 eV
Gap: 1.35 eV

(2)



Relative energy
2.7 kcal/mol
HOMO: –5.00 eV
LUMO: –3.86 eV
Gap: 1.14 eV

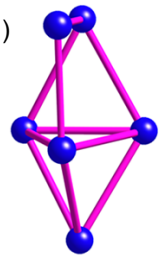
(3)



Relative energy
3.4 kcal/mol
HOMO: –5.32 eV
LUMO: –4.05 eV
Gap: 1.27 eV

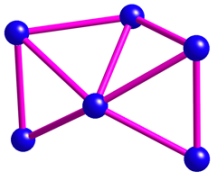
Pt_6

(1)



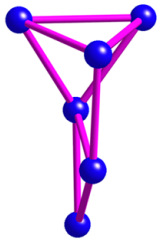
Relative energy
0 kcal/mol
HOMO: –5.71 eV
LUMO: –4.34 eV
Gap: 1.37 eV

(2)



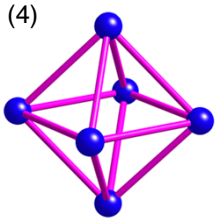
Relative energy
2.7 kcal/mol
HOMO: –5.83 eV
LUMO: –4.38 eV
Gap: 1.48 eV

(3)



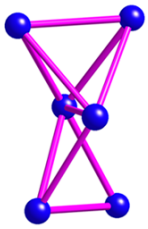
Relative energy
3.4 kcal/mol
HOMO: –5.58 eV
LUMO: –4.43 eV
Gap: 1.14 eV

(4)



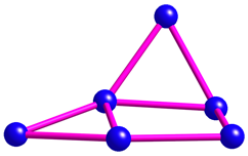
Relative energy
6.3 kcal/mol
HOMO: –5.20 eV
LUMO: –3.74 eV
Gap: 1.46 eV

(5)



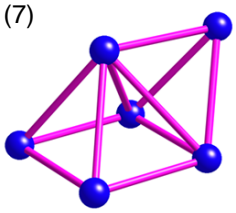
Relative energy
7.7 kcal/mol
HOMO: –5.53 eV
LUMO: –4.31 eV
Gap: 1.21 eV

(6)



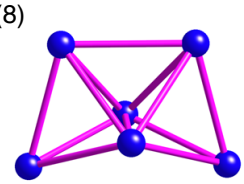
Relative energy
8.0 kcal/mol
HOMO: –5.85 eV
LUMO: –4.64 eV
Gap: 1.21 eV

(7)



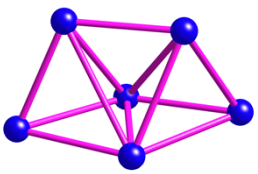
Relative energy
8.3 kcal/mol
HOMO: –5.27 eV
LUMO: –4.15 eV
Gap: 1.12 eV

(8)



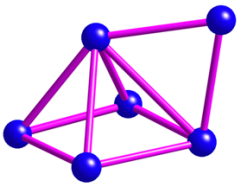
Relative energy
10.7 kcal/mol
HOMO: –5.28 eV
LUMO: –4.11 eV
Gap: 1.17 eV

(9)



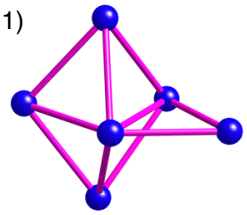
Relative energy
10.7 kcal/mol
HOMO: –5.41 eV
LUMO: –4.26 eV
Gap: 1.14 eV

(10)



Relative energy
10.7 kcal/mol
HOMO: –5.36 eV
LUMO: –4.43 eV
Gap: 1.14 eV

(11)



Relative energy
10.7 kcal/mol
HOMO: –5.25 eV
LUMO: –4.03 eV
Gap: 1.22 eV

Figure S2 Optimized geometries for Pt_6 and Pt_5 isomers.

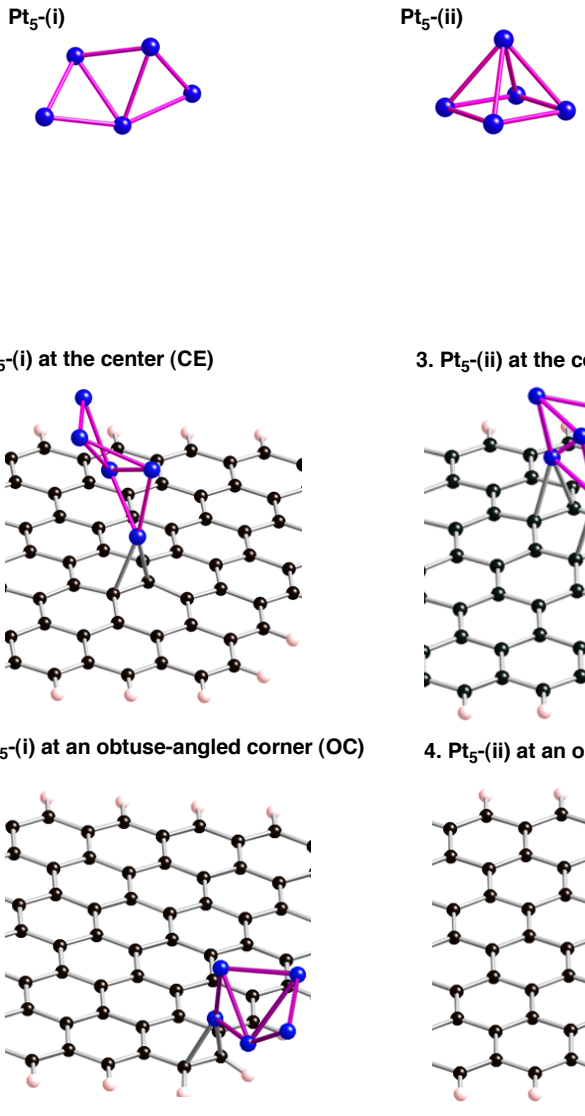


Fig. S3 Four optimized structures of Pt_5 clusters on $C_{96}H_{26}$. CE represents the center of $C_{96}H_{26}$, and OC represents an obtuse-angled corner. We can distinguish the four structures by Pt_5 cluster shapes as well as whetehr a Pt_5 cluster binds into an edge or the center of $C_{96}H_{26}$. The number of adsorbed Pt atoms (NAPt) can be also seen.

Table S1 Key geometrical parameters of a Pt_5 cluster on $C_{96}H_{26}$ and their energtics (kcal/mol).

	B3LYP (finite-size system)	
	Pt-C Bonds	E_{bind}[a]
1. Pt_5(i)-CE	2.253, 2.246	16.3
2 Pt_5(i)-OC	2.146, 2.154	35.9
3 Pt_5(ii)-CE	2.277, 2.274, 2.308, 2.314	22.2
4 Pt_5(ii)-OC	2.123, 2.123	10.0

[a] $E_{bind} = [E_{total}(Pt_5–C_{96}H_{26}) – E_{total}(C_{96}H_{26}) – E_{total}(Pt_5)] / NAPt$, where NAPt is the number of attached Pt atom listed in Fig. S3. With respect to the calculated binding energies, a counterpoise correction for basis set superposition error (BSSE) was included.