Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

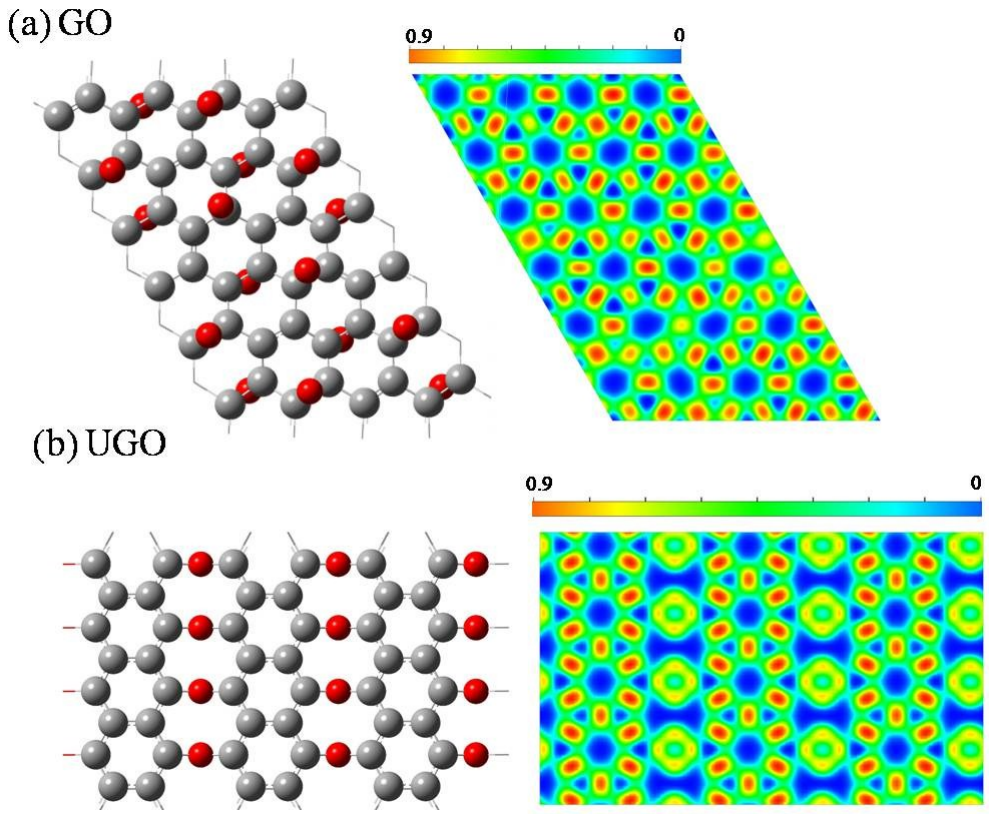

Figure S1. Top views of all calculated geometric structures and Electron localization function (ELF) plots of (a)GO and (b)UGO. The gray and red atoms represent carbon and oxygen, respectively.

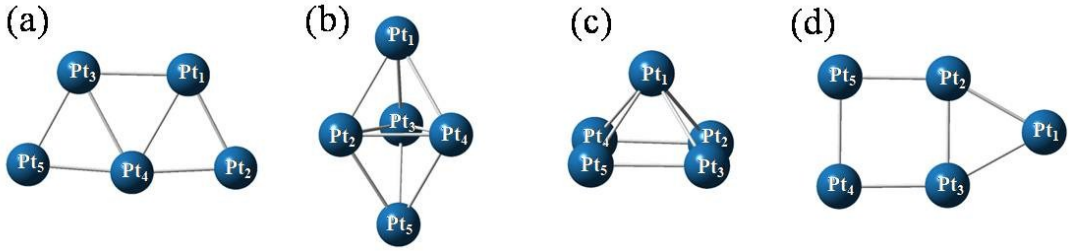

Figure S2. Side views of all calculated geometric structures of (a)Planer; (b)Triangular-dipyramid; (c)Pyramid and (d)flat.

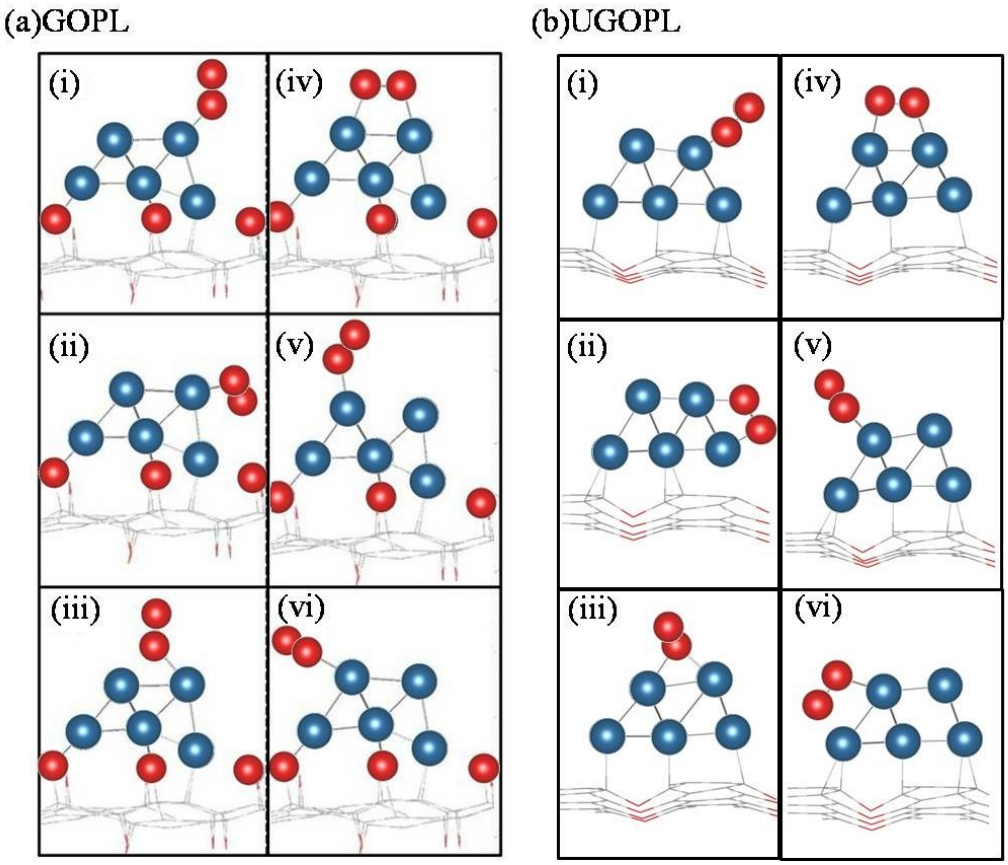

Figure S3. Side views of all most stable adsorption geometric structures of O_2 on (a) GOPL and (b)UGOPL systems.

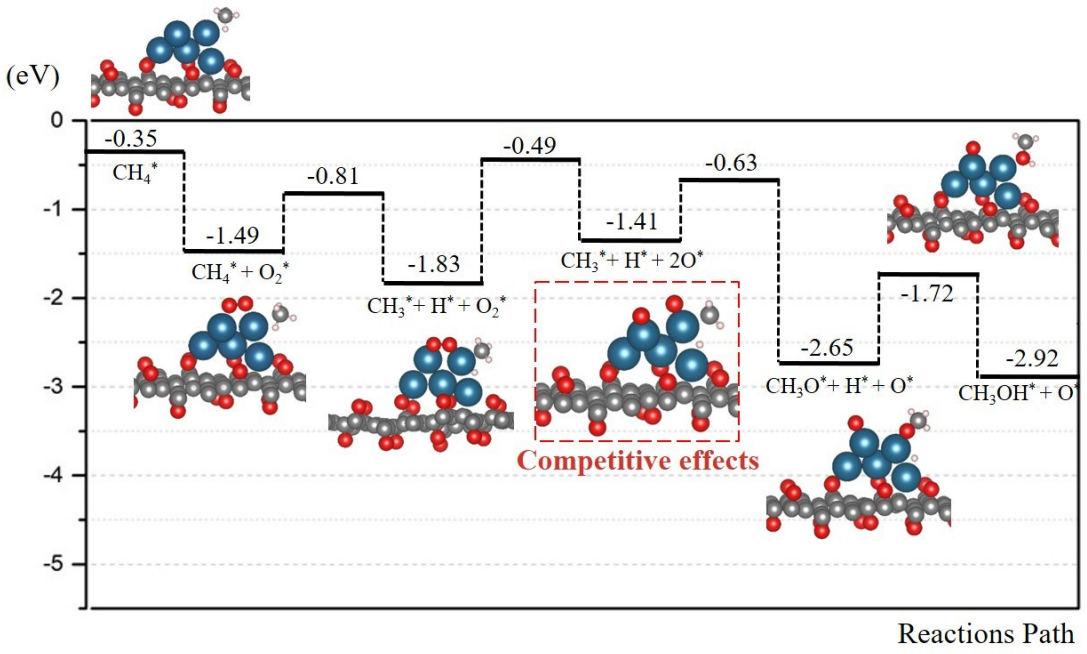

Figure S4. Profiles of the potential-energy surface for the methane conversion via L-H mechanism on GOPL system.

Table S1. Calculated relative energies of different Pt_5cluster(eV)

Pt_5cluster	Pt_5-flat	Pt_5-bipyramid	Pt_5-pyramid	Pt_5-planar
Singlet	0.17	0.20	0.22	0.12
Triplet	**0.00**	0.15	0.18	0.10
Quintet	0.16	**0.00**	0.12	**0.00**
Septet	0.26	0.42	**0.00**	0.07
Nonet	-	-	0.42	-

Table S2 Calculated Activation Energies (E_a) and Reaction Energies (ΔE) of methane conversion to methanol on Pt_2/GO[51] and GOPL

Pt_2/GO[51]					
Reaction Pathway I	E_a/eV	ΔE/eV	**Reaction Pathway II**	E_a/eV	ΔE/eV
$CH_4^* \rightarrow CH_3^* + H^*$	0.33	+0.06	$O_2^* + {}^* \rightarrow O_2^* + CH_4^*$	-	-0.24
$CH_3^* + H^* + O_{(GO)} \rightarrow CH_3^* + OH^*$	0.80	-1.24	$CH_4^* + O_2^* \rightarrow CH_3^* + OH^* + O^*$	0.72	-0.02
$CH_3^* + OH^* \rightarrow CH_3OH^*$	1.76	+0.29	$CH_3^* + OH^* + O^* \rightarrow CH_3OH^* + O^*$	0.71	-0.97
$CH_3OH^* \rightarrow CH_3OH_{(g)}$	-	+1.39	$CH_3OH^* + O^* \rightarrow CH_3OH_{(g)} + O^*$	-	+1.04
			$O^* + {}^* \rightarrow O^* + CH_4^*$	-	-0.46
			$CH_4^* + O^* \rightarrow CH_3^* + OH^*$	0.84	-0.99
			$CH_3^* + OH^* \rightarrow CH_3OH^*$	1.03	-0.17
			$CH_3OH^* \rightarrow CH_3OH_{(g)}$	-	+1.01
GOPL					
L-H mechanism	E_a/eV	ΔE/eV	**E-R mechanism**	E_a/eV	ΔE/eV
$CH_{4(g)} + {}^* \rightarrow CH_4^*$	-	-0.35	$O_2 + {}^* \rightarrow O_2^*$	-	-1.41
$CH_4^* + {}^* + O_{2(g)} \rightarrow CH_4^* + O_2^*$	-	-1.14	$CH_{4(g)} + O_2^* \rightarrow [CH_3 \cdot \cdot H] + 2O^*$	0.49	-1.07
$CH_4^* + O_2^* \rightarrow CH_3^* + H^* + O_2^*$	0.68	-1.32	$[CH_3 \cdot \cdot H] + 2O^* \rightarrow CH_3^* + OH^* + O^*$	0.94	-0.39
$CH_4^* + O_2^* \rightarrow CH_3^* + H^* + O^* + O^*$	1.34	+0.42	$CH_3^* + OH^* + O^* \rightarrow CH_3OH^* + O^*$	0.24	+1.04
$CH_3^* + H^* + O^* + O^* \rightarrow CH_3O^* + H^* + O^*$	0.78	-1.24	$CH_3OH^* + O^* \rightarrow CH_3OH_{(g)} + O^*$	-	+1.01
$CH_3O^* + H^* + O^* \rightarrow CH_3OH^* + O^*$	0.93	-0.27	$O^* + CH_{4(g)} \rightarrow O^* + CH_4^*$	-	-0.41
			$O^* + CH_4^* \rightarrow CH_3^* + H^* + O^*$	0.08	-0.85
			$CH_3^* + H^* + O^* \rightarrow CH_3O^* + H^*$	0.80	+0.02
			$CH_3O^* + H^* \rightarrow CH_3OH^*$	0.78	+0.30
			$CH_3OH^* \rightarrow CH_3OH_{(g)}$	-	+0.95

* = adsorption state