MS No.: CP-ART-03-2016-002134.R1

Optical Response and Gas Sequestration Properties of Metal Cluster Supported Graphene Nanoflakes

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Supplementary Information

Table

Table S1. Free energy change (ΔG, kcal/mol) and reaction enthalpy change (ΔH, kcal/mol) at 298K for the process: $CO/NO/CH_3OH$ + GR/BGR/BNGR → $CO/NO/CH_3OH$@GR/BGR/BNGR; ZPE corrected dissociation energy (D_0, kcal/mol) for the dissociation process: $CO/NO/CH_3OH$@GR/BGR/BNGR → $CO/NO/CH_3OH$ + GR/BGR/BNGR; HOMO-LUMO gap (Gap) (in eV), Polarizability (α) (in a.u.^{3}); most important stabilizing donor-acceptor interaction (*E(2)*) (in kcal/mol) as given by second order perturbation theory analysis of Fock matrix in the NBO basis for the $CO/NO/CH_3OH$@GR/BGR/BNGR moieties; NBO charges on adsorbate molecules (Q_K(Ad)); distance in between the adsorbates and adsorbent ($R_{Ad\text{-}Surface}$) (in Å); important bond lengths of the $CO/NO/CH_3OH$ molecules at the adsorbed state on $CO/NO/CH_3OH$ @GR/BGR/BNGR (in Å).

Systems	ΔG	ΔH	**D_0**	**Gap**	**α**	***E(2)***	**Q_K(Ad)**	**$R_{Ad\text{-}Surface}$**	**R_{Ad}**
CO@ GR	4.35	-3.05	3.47	3.95	684.19	$BD_{C\text{-}C}$ to LP^*_C =0.75	O=-0.51, C= 0.51	C-C= 3.29	C-O= 1.14

NO@ GR	-2.65	-9.23	9.77	4.68	628.09	LP_N to BD^*_{C-C} =0.24	N= 0.21, O= -0.20	N-C= 3.13	N-O= 1.15
CH_3OH@ GR	3.01	-6.27	6.72	3.96	688.30	BD_{C-C} to BD^*_{O-H} =0.78	O=-0.76, H_a=0.49, C=-0.32, H_b=0.22, 0.19, 0.19	O-C= 3.26, H_a-C= 2.60	O-H_a=0.96, C-O= 1.40, C-H_b= 1.10
CO@ BGR	3.92	-2.87	3.32	3.08	859.82	LP^*_C to LP^*_B =5.98	O=-0.51, C= 0.51	C-B= 3.25	C-O= 1.14
NO@ BGR	-13.50	-21.59	22.01	4.74	639.08	LP^*_B to BD^*_{N-O} =16.14	N= 0.24, O= -0.18	N-B= 2.93	N-O= 1.15
CH_3OH@ BGR	1.04	-8.71	9.02	3.13	847.91	BD_{C-C} to BD^*_{O-H} =1.19	O=-0.77, H_a=0.50, C=-0.32, H_b=0.21, 0.19, 0.19	H_a-C= 2.54, O-C= 3.47	O-H_a=0.96, C-O= 1.41, C-H_b= 1.09
CO@ BNGR	3.19	-2.94	3.45	3.67	705.99	LP^*_C to LP^*_B =5.60	O=-0.50, C= 0.51	C-N= 1.14	C-O= 1.14
NO@ BNGR	-8.74	-14.98	15.56	4.89	603.01	LP_N to BD^*_{B-N} =0.76	N= 0.20, O= -0.19	N-N= 2.96	N-O= 1.15
CH_3OH@ BNGR	1.03	-8.20	8.64	3.67	707.83	LP_O to BD^*_{C-H} =9.44	O=-0.76, H_a=0.49, C=-0.33, H_b=0.20, 0.20, 0.22	O-B= 3.00, H_a-B= 2.96	O-H_a=0.96, C-O= 1.42, C-H_b= 1.09

Table S2. NBO charges on M_3O^+ moieties ($Q_K(M_3O^+)$); distance in between the O/M centres of the M_3O^+ moieties from the host surface ($R_{M3O^+\text{-Surface}}$) (in Å) in the CO/NO/CH_3OH@M_3O^+GR/BGR/BNGR complexes.

Systems	**$Q_K(M_3O^+)$**	**$R_{M3O^+\text{-Surface}}$**
CO@ Li_3O^+GR	Q_{Li}=0.78, 0.74, 0.82 Q_O=-1.01	Li-C= 2.49
NO@ Li_3O^+GR	Q_{Li}=0.81, 0.88, 0.78 Q_O=-0.98	Li-C= 2.49
CH_3OH@ Li_3O^+GR	Q_{Li}=0.81, 0.80, 0.80 Q_O=-1.52	Li-C= 2.57
CO@ Na_3O^+GR	Q_{Na}=0.81, 0.79, 0.83 Q_O=-1.02	Na-C= 2.78
NO@ Na_3O^+GR	Q_{Na}=0.90, 0.87, 0.90 Q_O=-0.57	Na-C= 2.69
CH_3OH@ Na_3O^+GR	Q_{Na}=0.87, 0.86, 0.81 Q_O=-1.58	Na-C= 2.85
CO@ K_3O^+GR	Q_K=0.81, 0.83, 0.82 Q_O=-0.97	O-C= 2.96
NO@ K_3O^+GR	Q_K=0.89, 0.92, 0.93 Q_O=-0.66	K-C= 2.99
CH_3OH@ K_3O^+GR	Q_K=0.85, 0.82, 0.86 Q_O=-1.53	K-C= 3.20
CO@ Li_3O^+BGR	Q_{Li}=0.90, 0.81, 0.72 Q_O=-1.23	O-B= 1.58, Li-C_{Avg}= 2.43
NO@ Li_3O^+BGR	Q_{Li}=0.89, 0.82, 0.79 Q_O=-1.26	O-B= 1.59, Li-C_{Avg}= 2.45
CH_3OH@ Li_3O^+BGR	Q_{Li}=0.89, 0.80, 0.85 Q_O=-1.23	O-B= 1.57, Li-C_{Avg}= 2.37
CO@ Na_3O^+BGR	Q_{Na}=0.91, 0.88, 0.83 Q_O=-1.58	O-B= 1.55, Na-C_{Avg}= 2.49
NO@ Na_3O^+BGR	Q_{Na}=0.93, 0.87, 0.88 Q_O=-1.25	O-B= 1.53, Na-C_{Avg}= 2.55
CH_3OH@ Na_3O^+BGR	Q_{Na}=0.91, 0.89, 0.92 Q_O=-1.23	O-B= 1.54, Na-C_{Avg}= 2.51
CO@ K_3O^+BGR	Q_K=0.88, 0.90, 0.91 Q_O=-1.16	O-B= 1.52, K-C_{Avg}= 2.81
NO@ K_3O^+BGR	Q_K=0.89, 0.92, 0.92 Q_O=-0.56	O-B= 3.84, K-C_{Avg}= 3.00
CH_3OH@ K_3O^+BGR	Q_K=0.92, 0.93, 0.90 Q_O=-1.18	O-B= 1.51, K-C_{Avg}= 2.80
CO@ Li_3O^+BNGR	Q_{Li}=0.89, 0.90, 0.70 Q_O=-1.29	O-B= 1.54, Li-N_{Avg}= 2.14, Li-C= 2.16
NO@ Li_3O^+BNGR	Q_{Li}=0.82, 0.89, 0.82 Q_O=-1.30	O-B= 1.53, Li-N_{Avg}= 2.12, Li-C= 2.21
CH_3OH@Li_3O^+BNGR	Q_{Li}=0.82, 0.90, 0.84 Q_O=-1.30	O-B= 1.53, Li-N_{Avg}= 2.13, Li-C= 2.29
CO@ Na_3O^+BNGR	Q_{Na}=0.92, 0.87, 0.83 Q_O=-1.27	O-B= 1.48, Na-N_{Avg}= 2.47, Na-C= 2.47
NO@ Na_3O^+BNGR	Q_{Na}=0.93, 0.88, 0.86 Q_O=-1.26	O-B= 1.46, Na-N_{Avg}= 2.52, Na-C= 2.65
CH_3OH@Na_3O^+BNGR	Q_{Na}=0.93, 0.89, 0.88 Q_O=-1.27	O-B= 1.48, Na-N_{Avg}= 2.48, Na-C= 2.55
CO@	Q_K=0.91, 0.88, 0.90	O-B= 1.45, K-N_{avg}= 2.82, K-C=

K_3O^+BNGR	Q_O=-1.22	2.81
NO@K_3O^+BNGR	Q_K=0.92, 0.92, 0.93 Q_O=-0.74	O-B= 1.54, K-N= 2.94, K-C= 2.96
CH_3OH@K_3O^+BNGR	Q_K=0.91, 0.90, 0.94 Q_O=-1.23	O-B= 1.44, K-N_{avg}= 2.84, K-C= 2.85

Table S3. Electron density descriptors (in a.u.) at the bond critical points (BCP) for the CO/NO/CH_3OH@M_3O^+GR/BGR/BNGR moieties. Herein, subscripts MOL-G, M-G, MOL-M, MOL refer to the BCPs belonging to the adsorbate-GR/BGR/BNGR, M_3O^+-GR/BGR/BNGR, adsorbate- M_3O^+ and adsorbate moieties respectively.

Systems	**BCP**	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$H(r_c)$	$-G(r_c)/V(r_c)$	**ELF**
CO@GR	O-C_{MOL-G}	0.00	0.02	0.00	1.28	0.01
	C-C_{MOL-G}	0.01	0.02	0.00	1.39	0.02
	C-O_{MOL}	0.47	1.45	-0.76	0.59	0.35
NO@GR	O-C_{MOL-G}	0.01	0.02	0.00	1.23	0.01
	N-C_{MOL-G}	0.01	0.03	0.00	1.19	0.04
	N-O_{MOL}	0.58	-2.07	-1.09	0.35	0.80
CH_3OH@GR	H-C_{MOL-G}	0.01	0.03	0.00	1.30	0.03
	O-C_{MOL-G}	0.01	0.02	0.00	1.22	0.02
	O-H_{MOL}	0.37	-2.11	-0.61	0.12	0.98
	C-O_{MOL}	0.26	-0.47	-0.39	0.41	0.57
CO@BGR	C-C_{MOL-G}	0.01	0.02	0.00	1.37	0.03
	O-C_{MOL-G}	0.00	0.01	0.00	1.30	0.01
	C-O_{MOL}	0.47	1.44	-0.76	0.60	0.35
NO@BGR	N-C_{MOL-G}	0.01	0.03	0.00	1.07	0.07
	O-C_{MOL-G}	0.01	0.02	0.00	1.19	0.02
	N-O_{MOL}	0.58	-2.13	-1.12	0.35	0.80
CH_3OH@BGR	C-C_{MOL-G}	0.01	0.02	0.00	1.32	0.02

	$H\text{-}C_{MOL\text{-}G}$	0.01	0.03	0.00	1.25	0.03
	$C\text{-}O_{MOL}$	0.27	-0.49	-0.39	0.41	0.58
	$O\text{-}H_{MOL}$	0.37	-2.12	-0.61	0.11	0.98
CO@BNGR	$C\text{-}N_{MOL\text{-}G}$	0.01	0.03	0.00	1.29	0.03
	$C\text{-}O_{MOL}$	0.47	1.44	-0.77	0.60	0.35
NO@BNGR	$N\text{-}N_{MOL\text{-}G}$	0.01	0.03	0.00	1.22	0.03
	$N\text{-}O_{MOL}$	0.58	-2.07	-1.09	0.34	0.80
CH_3OH@BNGR	$O\text{-}N_{MOL\text{-}G}$	0.01	0.03	0.00	1.06	0.03
	$C\text{-}N_{MOL\text{-}G}$	0.01	0.03	0.00	1.27	0.02
	$C\text{-}O_{MOL}$	0.26	-0.44	-0.38	0.42	0.56
	$O\text{-}H_{MOL}$	0.37	-2.11	-0.61	0.12	0.98
CO@Li_3O^+GR	$O\text{-}C_{M\text{-}G}$	0.01	0.04	0.00	1.06	0.05
	$Li\text{-}C_{M\text{-}G}$	0.01	0.05	0.00	1.28	0.01
	$C\text{-}O_{MOL}$	0.38	0.09	-0.63	0.51	0.43
	$C\text{-}O_{MOL\text{-}M}$	0.26	-0.33	-0.38	0.44	0.51
	$O\text{-}Li_{MOL\text{-}M}$	0.04	0.27	0.00	1.27	0.04
NO@Li_3O^+GR	$O\text{-}C_{M\text{-}G}$	0.01	0.04	0.00	1.06	0.04
	$Li\text{-}C_{M\text{-}G}$	0.01	0.05	0.00	1.30	0.02
	$N\text{-}O_{MOL}$	0.37	-0.61	-0.40	0.38	0.83
	$N\text{-}O_{MOL\text{-}M}$	0.29	-0.24	-0.25	0.43	0.78
	$O\text{-}Li_{MOL\text{-}M}$	0.03	0.24	0.00	1.27	0.03
CH_3OH@ Li_3O^+GR	$O\text{-}C_{M\text{-}G}$	0.01	0.03	0.00	1.04	0.05
	$Li\text{-}C_{M\text{-}G}$	0.01	0.04	0.00	1.31	0.01
	$C\text{-}O_{MOL}$	0.24	-0.31	-0.35	0.44	0.51
	$O\text{-}H_{MOL}$	0.36	-2.15	-0.61	0.11	0.98
	$O\text{-}Li_{MOL\text{-}M}$	0.03	0.19	0.01	1.32	0.03

	H-C_{MOL-G}	0.01	0.03	0.00	1.19	0.04
CO@Na_3O^+GR	O-C_{M-G}	0.01	0.05	0.00	1.13	0.04
	Na-C_{M-G}	0.07	0.03	0.00	1.26	0.01
	C-O_{MOL}	0.35	-0.02	-0.57	0.50	0.44
	C-O_{MOL-M}	0.31	-0.25	-0.48	0.47	0.47
	O-Na_{MOL-M}	0.02	0.11	0.00	1.19	0.03
NO@Na_3O^+GR	O-C_{M-G}	0.01	0.02	0.00	1.16	0.02
	Na-C_{M-G}	0.01	0.07	0.00	1.26	0.02
	N-O_{MOL}	0.46	-1.03	-0.59	0.36	0.85
	N-O_{MOL-M}	0.47	-1.04	-0.59	0.36	0.85
CH_3OH@	O-C_{M-G}	0.01	0.02	0.00	1.17	0.04
Na_3O^+GR	Na-C_{M-G}	0.01	0.03	0.00	1.28	0.01
	C-O_{MOL}	0.24	-0.28	-0.34	0.44	0.50
	H-O_{MOL}	0.37	-2.15	-0.62	0.11	0.98
	O-Na_{MOL-M}	0.02	0.15	0.01	1.27	0.03
	H-O_{MOL-M}	0.02	0.05	0.00	0.90	0.11
CO@K_3O^+GR	O-C_{M-G}	0.01	0.04	0.00	1.14	0.03
	K-C_{M-G}	0.01	0.03	0.00	1.36	0.02
	C-O_{MOL}	0.35	-0.02	-0.56	0.50	0.44
	C-O_{MOL-M}	0.31	-0.20	-0.49	0.47	0.46
	O-K_{MOL-M}	0.02	0.09	0.00	1.10	0.05
NO@	O-C_{M-G}	0.00	0.01	0.00	1.30	0.01
K_3O^+GR	K-C_{M-G}	0.02	0.08	0.00	1.11	0.04
	N-O_{MOL}	0.50	-1.20	-0.67	0.36	0.85
	N-O_{MOL-M}	0.43	-0.86	-0.52	0.37	0.85
CH_3OH@	O-C_{M-G}	0.01	0.02	0.00	1.29	0.03

K_3O^+GR	K-C_{M-G}	0.01	0.03	0.00	1.34	0.02
	H-O_{MOL-M}	0.03	0.06	0.00	0.86	0.16
	O-K_{MOL-M}	0.02	0.09	0.00	1.14	0.04
	O-H_{MOL}	0.37	-2.13	-0.61	0.12	0.98
	C-O_{MOL}	0.24	-0.30	-0.34	0.44	0.50
CO@	O-B_{M-G}	0.12	0.40	-0.08	0.69	0.18
Li_3O^+BGR	Li-C_{M-G}	0.02	0.07	0.00	1.19	0.03
	C-O_{MOL}	0.48	1.44	-0.79	0.59	0.35
	C-Li_{MOL-M}	0.01	0.07	0.00	1.48	0.02
	C-C_{MOL-G}	0.01	0.02	0.00	1.33	0.03
NO@	O-B_{M-G}	0.12	0.39	-0.08	0.69	0.18
Li_3O^+BGR	Li-C_{M-G}	0.01	0.06	0.00	1.32	0.02
	N-O_{MOL}	0.57	-2.02	-1.06	0.34	0.81
	O-Li_{MOL-M}	0.01	0.04	0.00	1.35	0.01
	N-O_{MOL-M}	0.01	0.02	0.00	1.05	0.03
CH_3OH@	O-B_{M-G}	0.12	0.41	-0.08	0.70	0.18
Li_3O^+BGR	Li-C_{M-G}	0.02	0.10	0.00	1.25	0.04
	O-H_{MOL}	0.37	-2.18	-0.62	0.11	0.98
	C-O_{MOL}	0.24	-0.25	-0.34	0.45	0.48
	O-Li_{MOL-M}	0.03	0.23	0.00	1.35	0.03
	H-C_{MOL-G}	0.01	0.02	0.00	1.31	0.03
CO@	O-B_{M-G}	0.13	0.44	-0.09	0.70	0.19
Na_3O^+BGR	Na-C_{M-G}	0.02	0.09	0.00	1.26	0.03
	C-O_{MOL}	0.47	1.35	-0.78	0.59	0.35
	C-Na_{MOL-M}	0.01	0.04	0.00	1.38	0.01
	C-O_{MOL-M}	0.01	0.02	0.00	1.23	0.03

	C-C_{MOL-G}	0.01	0.02	0.00	1.42	0.02
NO@	O-B_{M-G}	0.13	0.48	-0.09	0.70	0.19
Na_3O^+BGR	Na-C_{MOL-G}	0.02	0.08	0.00	1.28	0.03
	N-O_{MOL}	0.52	-1.61	-0.86	0.35	0.81
	O-C_{MOL-G}	0.01	0.03	0.00	1.11	0.04
	N-C_{MOL-G}	0.03	0.07	0.00	1.09	0.20
	N-Na_{MOL-M}	0.01	0.05	0.00	1.21	0.01
CH_3OH@	O-B_{M-G}	0.13	0.45	-0.09	0.70	0.19
Na_3O^+BGR	Na-C_{MOL-G}	0.02	0.09	0.00	1.27	0.03
	C-O_{MOL}	0.25	-0.34	-0.35	0.43	0.52
	O-H_{MOL}	0.36	-2.14	-0.61	0.11	0.98
	O-Na_{MOL-M}	0.02	0.15	0.01	1.24	0.03
	H-C_{MOL-G}	0.01	0.04	0.00	1.16	0.05
CO@	O-B_{M-G}	0.14	0.49	-0.09	0.70	0.20
K_3O^+BGR	K-C_{M-G}	0.02	0.07	0.00	1.24	0.04
	C-O_{MOL}	0.47	1.33	-0.77	0.59	0.35
	C-O_{MOL-M}	0.01	0.04	0.00	1.11	0.06
	O-K_{MOL-M}	0.01	0.04	0.00	1.38	0.02
NO@	K-C_{M-G}	0.01	0.04	0.00	1.27	0.03
K_3O^+BGR	N-O_{MOL}	0.47	-1.03	-0.59	0.36	0.85
	N-O_{MOL-M}	0.46	-1.03	-0.59	0.36	0.85
	O-K_{MOL-M}	0.02	0.01	0.00	1.11	0.05
CH_3OH@	O-B_{M-G}	0.14	0.49	-0.09	0.70	0.20
K_3O^+BGR	K-C_{M-G}	0.02	0.07	0.00	1.24	0.04
	C-O_{MOL}	0.25	-0.38	-0.37	0.42	0.54
	O-H_{MOL}	0.37	-2.15	-0.61	0.11	0.98

	$O\text{-}K_{MOL\text{-}M}$	0.02	0.08	0.00	1.13	0.04
	$H\text{-}O_{MOL}\text{-}_M$	0.02	0.04	0.00	0.97	0.06
CO@	$O\text{-}B_{M\text{-}G}$	0.13	0.45	-0.09	0.69	0.20
Li_3O^+BNGR	$Li\text{-}C_{M\text{-}G}$	0.02	0.12	0.01	1.24	0.03
	$C\text{-}O_{MOL}$	0.48	1.43	-0.80	0.59	0.35
	$C\text{-}Li_{MOL\text{-}M}$	0.01	0.08	0.01	1.44	0.02
	$C\text{-}C_{MOL\text{-}G}$	0.01	0.02	0.00	1.36	0.04
NO@	$O\text{-}B_{M\text{-}G}$	0.14	0.46	-0.09	0.69	0.20
Li_3O^+BNGR	$Li\text{-}C_{M\text{-}G}$	0.02	0.10	0.00	1.25	0.03
	$N\text{-}O_{MOL}$	0.57	-1.96	-1.02	0.34	0.81
	$O\text{-}Li_{MOL\text{-}M}$	0.01	0.06	0.00	1.35	0.01
	$N\text{-}Li_{MOL\text{-}M}$	0.01	0.05	0.00	1.34	0.01
	$N\text{-}O_{MOL\text{-}M}$	0.01	0.02	0.00	1.02	0.04
CH_3OH@	$O\text{-}B_{M\text{-}G}$	0.14	0.47	-0.09	0.69	0.20
Li_3O^+BNGR	$Li\text{-}C_{M\text{-}G}$	0.02	0.12	0.01	1.28	0.02
	$C\text{-}O_{MOL}$	0.25	-0.36	-0.36	0.43	0.53
	$O\text{-}H_{MOL}$	0.36	-2.14	-0.61	0.10	0.98
	$O\text{-}Li_{MOL\text{-}M}$	0.03	0.20	0.01	1.31	0.03
	$H\text{-}C_{MOL\text{-}G}$	0.01	0.03	0.00	1.15	0.04
CO@	$O\text{-}B_{M\text{-}G}$	0.15	0.56	-0.10	0.70	0.21
Na_3O^+BNGR	$Na\text{-}C_{M\text{-}G}$	0.02	0.09	0.00	1.23	0.03
	$C\text{-}O_{MOL}$	0.47	1.37	-0.78	0.59	0.35
	$C\text{-}Na_{MOL\text{-}M}$	0.01	0.05	0.00	1.38	0.01
	$O\text{-}Na_{MOL\text{-}M}$	0.00	0.02	0.00	1.44	0.00
NO@	$O\text{-}B_{M\text{-}G}$	0.16	0.62	-0.11	0.71	0.21
Na_3O^+BNGR	$Na\text{-}C_{M\text{-}G}$	0.02	0.09	0.00	1.24	0.02

	$N\text{-}O_{MOL}$	0.53	-1.59	-0.87	0.35	0.82
	$N\text{-}C_{MOL\text{-}G}$	0.02	0.05	0.00	1.20	0.09
	$O\text{-}C_{MOL\text{-}G}$	0.02	0.06	0.00	1.22	0.05
	$N\text{-}Na_{MOL\text{-}M}$	0.02	0.09	0.00	1.35	0.02
CH_3OH@	$O\text{-}B_{M\text{-}G}$	0.16	0.58	-0.11	0.70	0.21
Na_3O^+BNGR	$Na\text{-}C_{M\text{-}G}$	0.02	0.09	0.00	1.24	0.02
	$C\text{-}O_{MOL}$	0.26	-0.41	-0.37	0.42	0.55
	$O\text{-}H_{MOL}$	0.36	-2.11	-0.60	0.11	0.98
	$O\text{-}Na_{MOL\text{-}M}$	0.02	0.14	0.01	1.24	0.03
CO@	$O\text{-}B_{M\text{-}G}$	0.17	0.65	-0.11	0.71	0.22
K_3O^+BNGR	$K\text{-}C_{M\text{-}G}$	0.02	0.07	0.00	1.20	0.04
	$C\text{-}O_{MOL}$	0.47	1.32	-0.77	0.59	0.35
	$C\text{-}K_{MOL\text{-}M}$	0.01	0.04	0.00	1.38	0.02
	$C\text{-}O_{MOL\text{-}M}$	0.02	0.05	0.00	1.09	0.06
NO@	$O\text{-}B_{M\text{-}G}$	0.13	0.46	-0.08	0.71	0.18
K_3O^+BNGR	$K\text{-}C_{M\text{-}G}$	0.01	0.05	0.00	1.27	0.03
	$N\text{-}O_{MOL}$	0.42	-0.82	-0.49	0.37	0.85
	$O\text{-}K_{MOL\text{-}M}$	0.02	0.09	0.00	1.10	0.04
	$N\text{-}O_{MOL\text{-}M}$	0.28	-0.22	-0.24	0.43	0.78
CH_3OH@	$O\text{-}B_{M\text{-}G}$	0.17	0.70	-0.12	0.71	0.22
K_3O^+BNGR	$K\text{-}C_{M\text{-}G}$	0.02	0.07	0.00	1.21	0.03
	$C\text{-}O_{MOL}$	0.24	-0.32	-0.34	0.43	0.52
	$O\text{-}H_{MOL}$	0.37	-2.13	-0.61	0.11	0.98
	$O\text{-}K_{MOL\text{-}M}$	0.01	0.06	0.00	1.13	0.03
	$H\text{-}C_{MOL\text{-}G}$	0.01	0.03	0.00	1.22	0.04

Figures

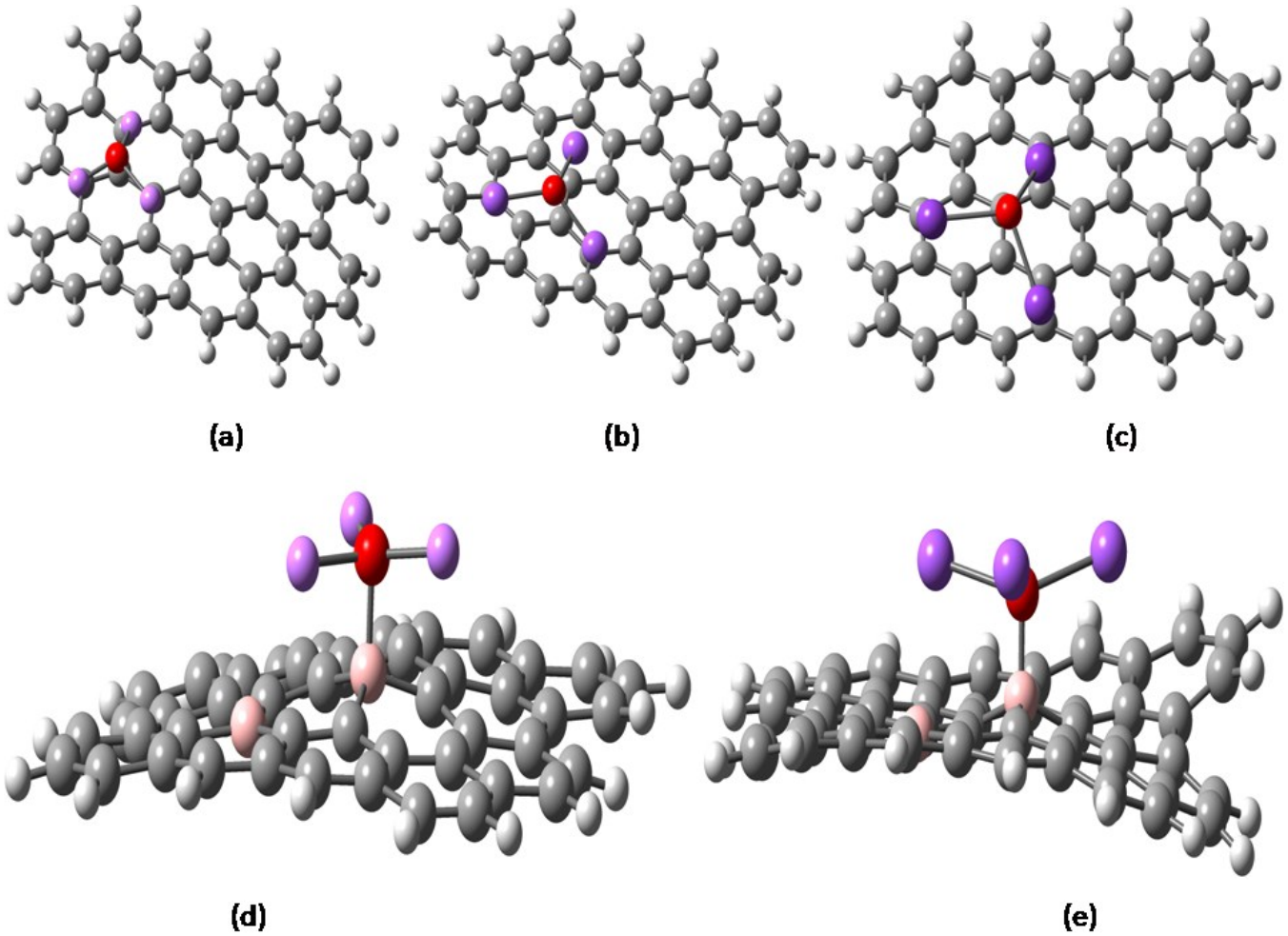

Figure S1: Geometrical alignment of the adsorbed guest@GR/BGR moieties at 500 fs where (a) Li_3O^+@GR, (b) Na_3O^+@GR, (c) K_3O^+@GR, (d) Li_3O^+@BGR and (e) Na_3O^+@BGR respectively.

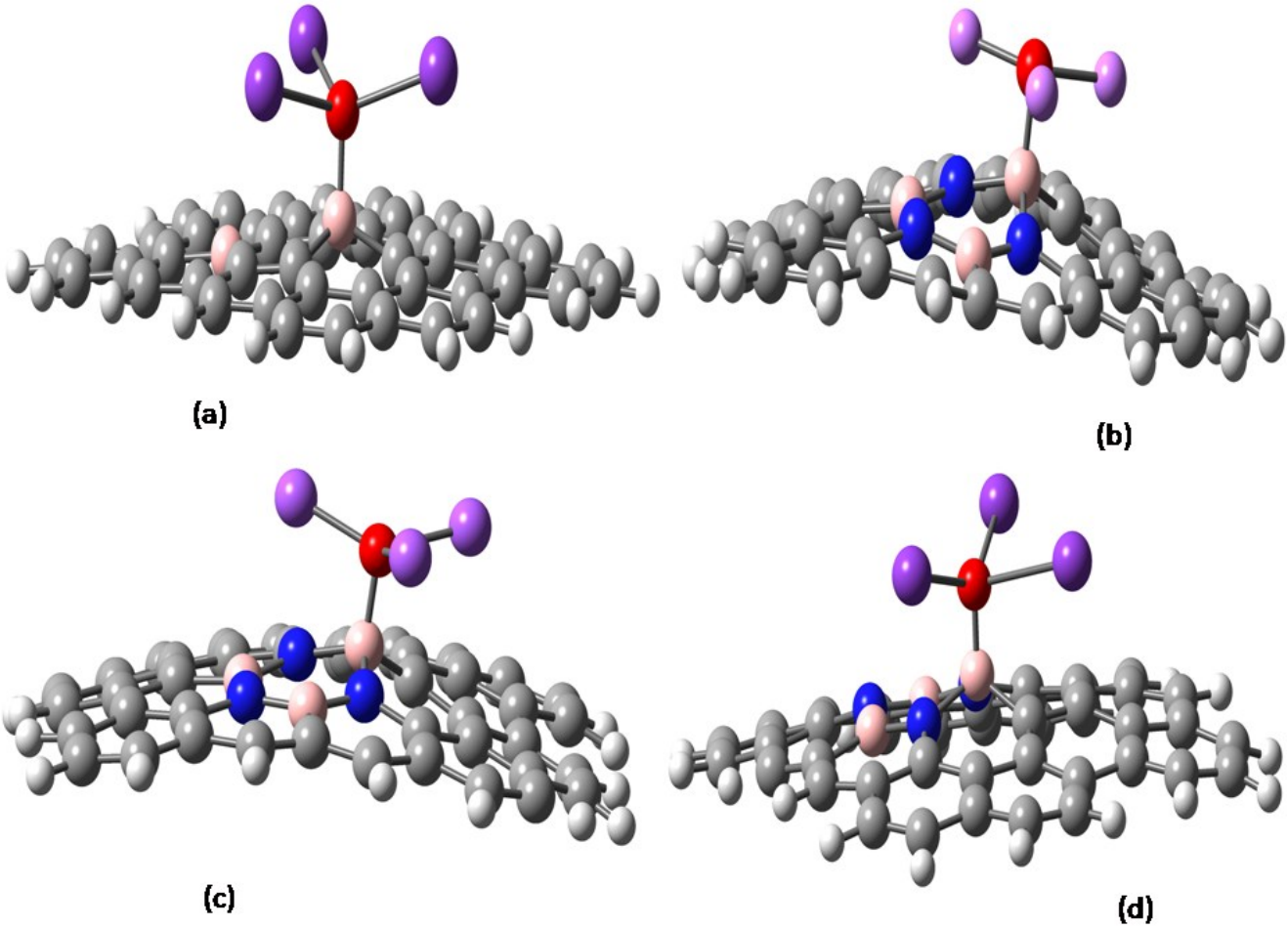

Figure S2: Geometrical alignment of the adsorbed guest@BGR/BNGR moieties at 500 fs where (a) K_3O^+@BGR, (b) Li_3O^+@BNGR, (c) Na_3O^+@BNGR and (d) K_3O^+@BNGR respectively.

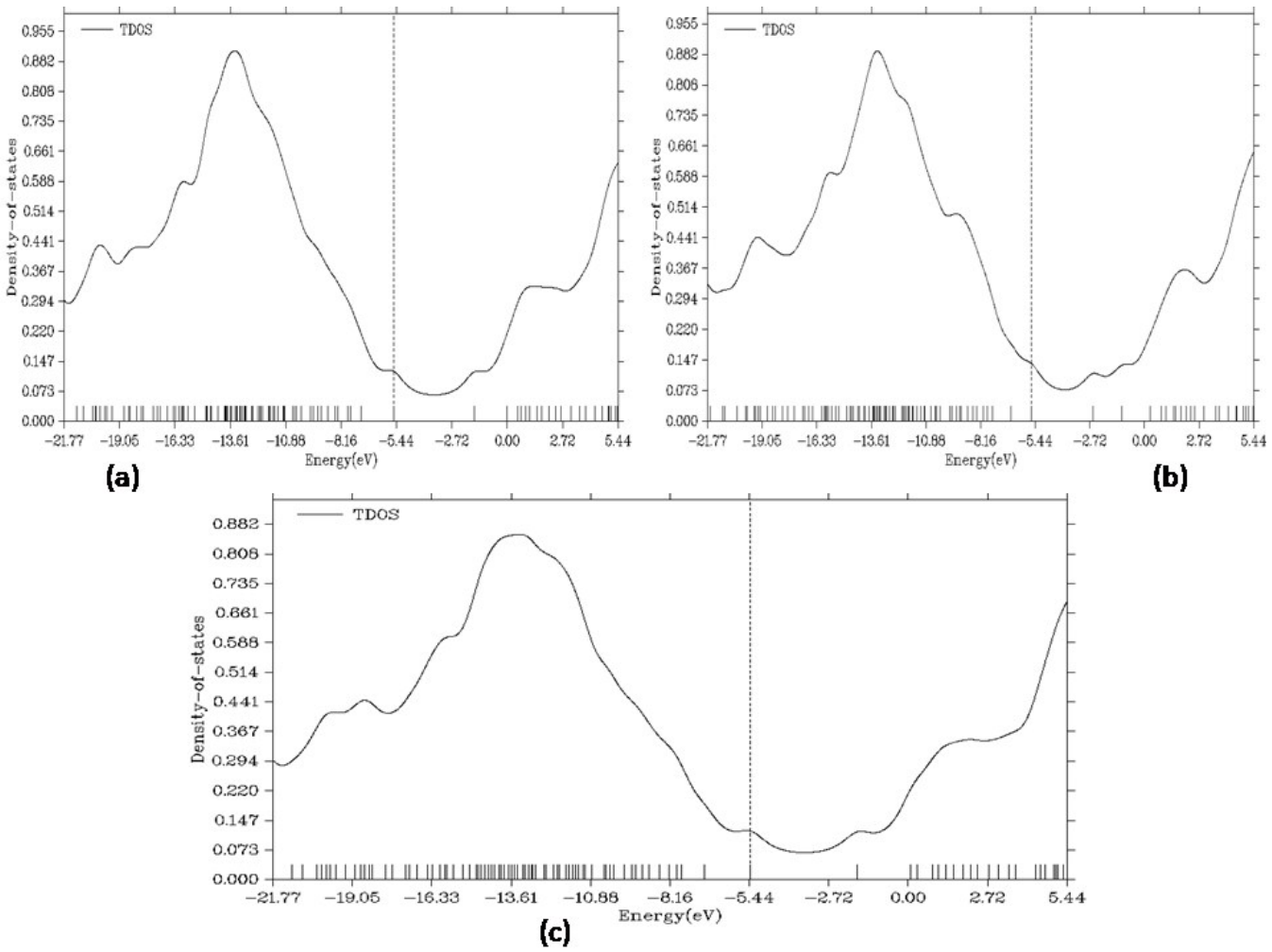

Figure S3. The TDOS plots of (a) GR, (b) BGR and (c) BNGR respectively.

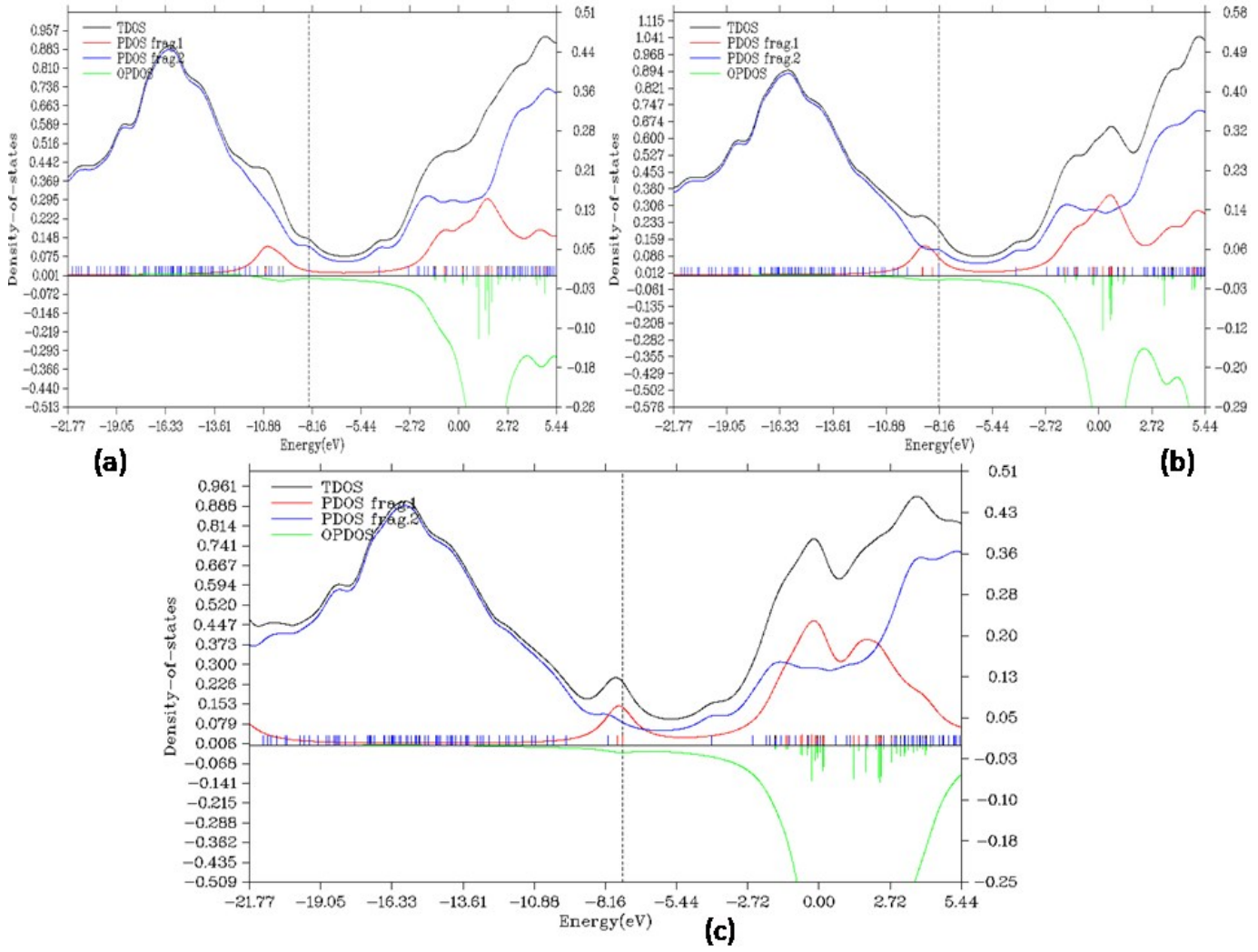

Figure S4. The TDOS plots of M_3O^+@GR where (a) Li_3O^+@GR, (b) Na_3O^+@GR and (c) K_3O^+@GR respectively. Here frag1 denotes M_3O^+ moieties whereas frag2 denotes GR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

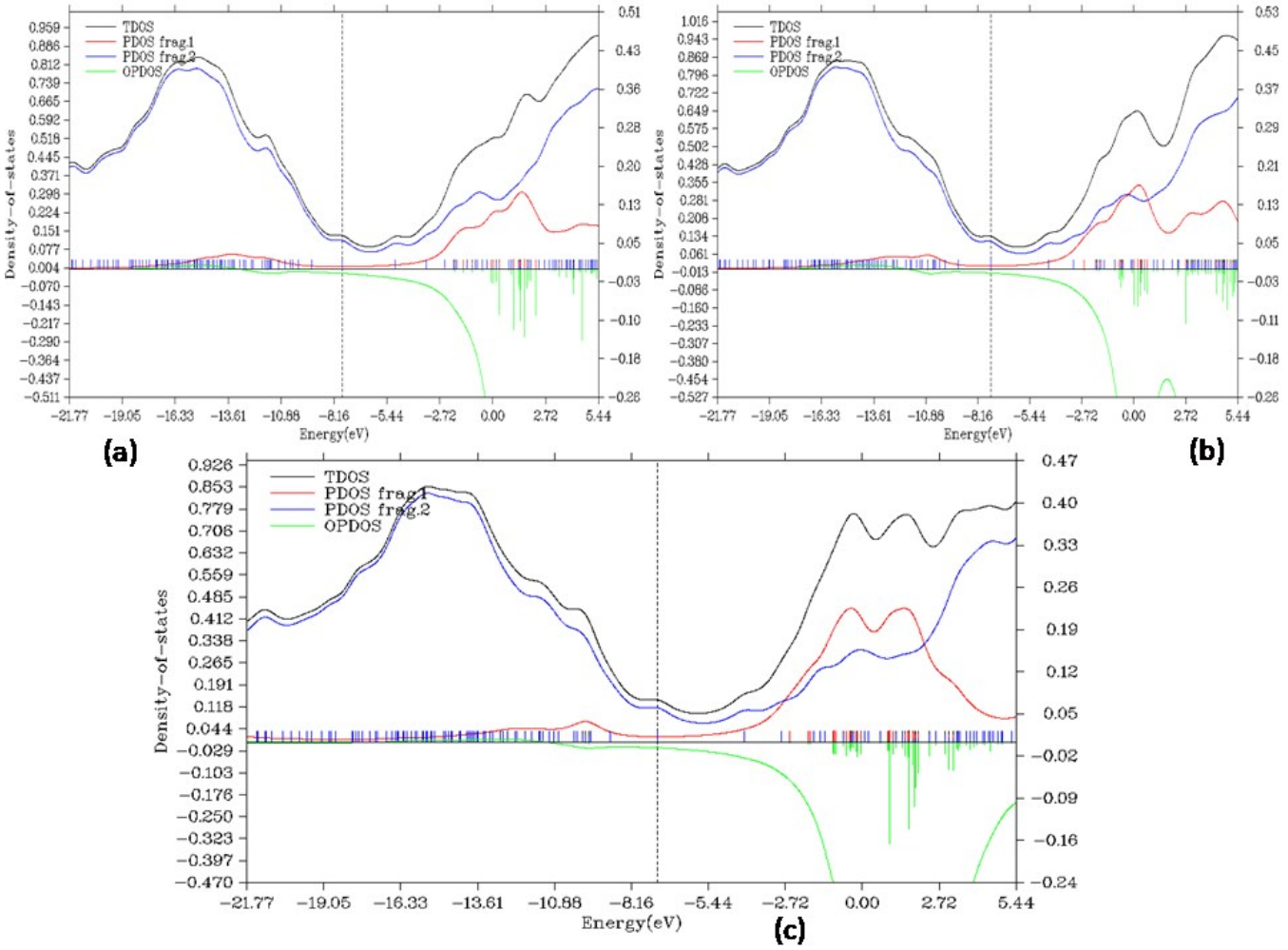

Figure S5. The TDOS plots of M_3O^+@BGR where (a) Li_3O^+@BGR, (b) Na_3O^+@BGR and (c) K_3O^+@BGR respectively. Here frag1 denotes M_3O^+ moieties whereas frag2 denotes BGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

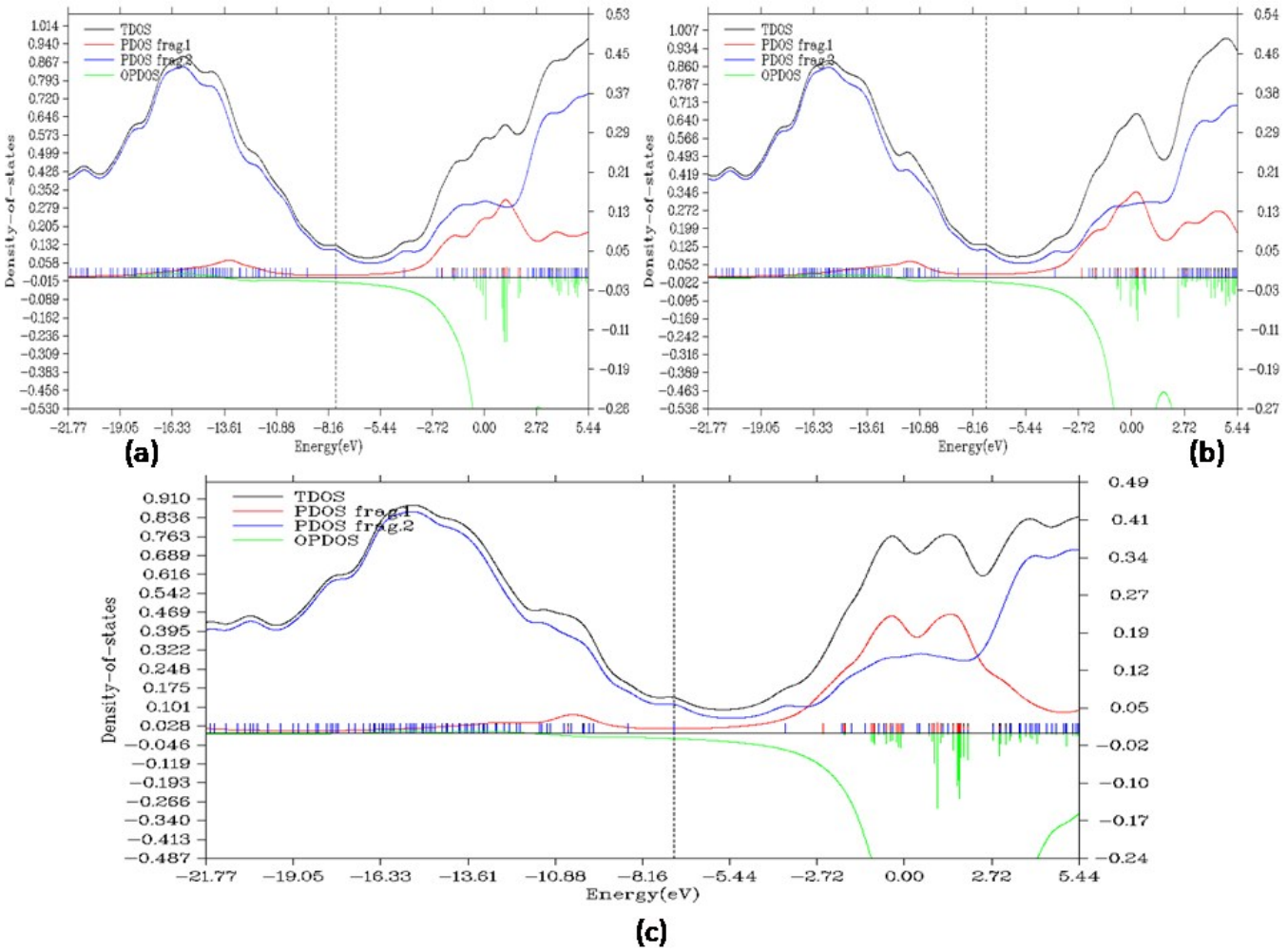

Figure S6. The TDOS plots of M_3O^+@BNGR where (a) Li_3O^+@BNGR, (b) Na_3O^+@BNGR and (c) K_3O^+@BNGR respectively. Here frag1 denotes M_3O^+ moieties whereas frag2 denotes BNGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

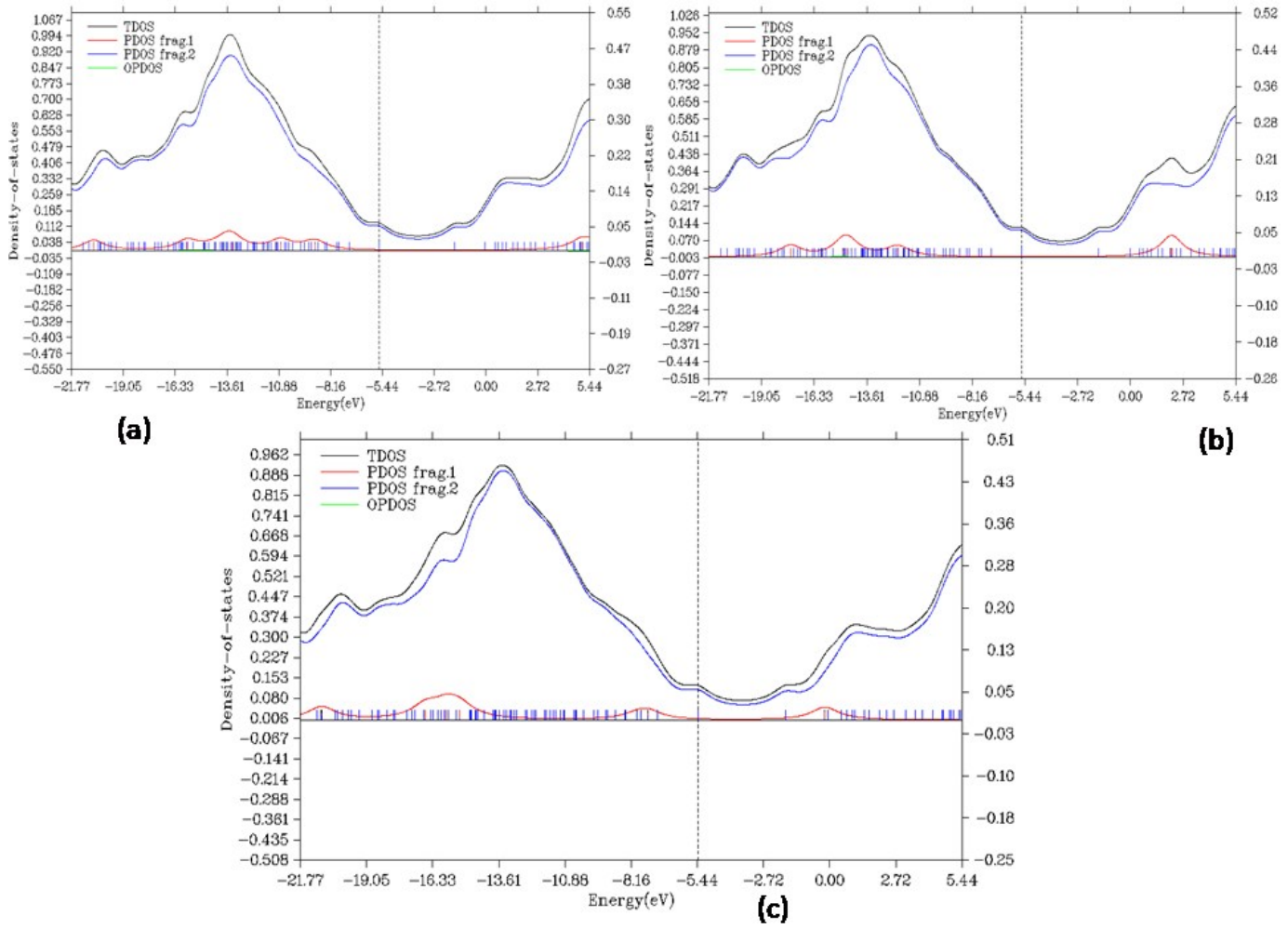

Figure S7. The TDOS plots of CO/NO/CH_3OH@GR where (a) CH_3OH@GR, (b) CO@GR and (c) NO@GR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes GR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

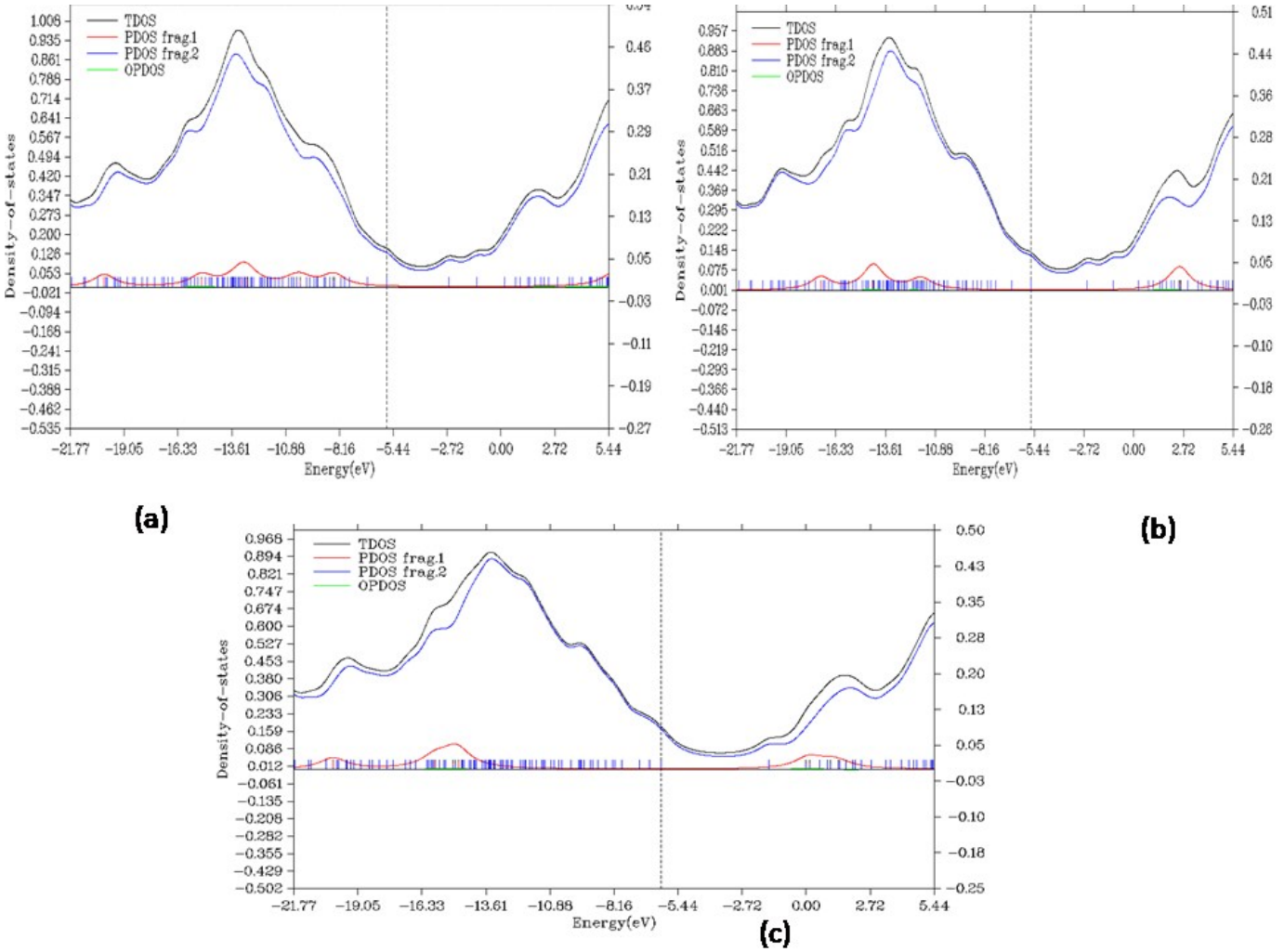

Figure S8. The TDOS plots of CO/NO/CH_3OH@BGR where (a) CH_3OH@BGR, (b) CO@BGR and (c) NO@BGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes BGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

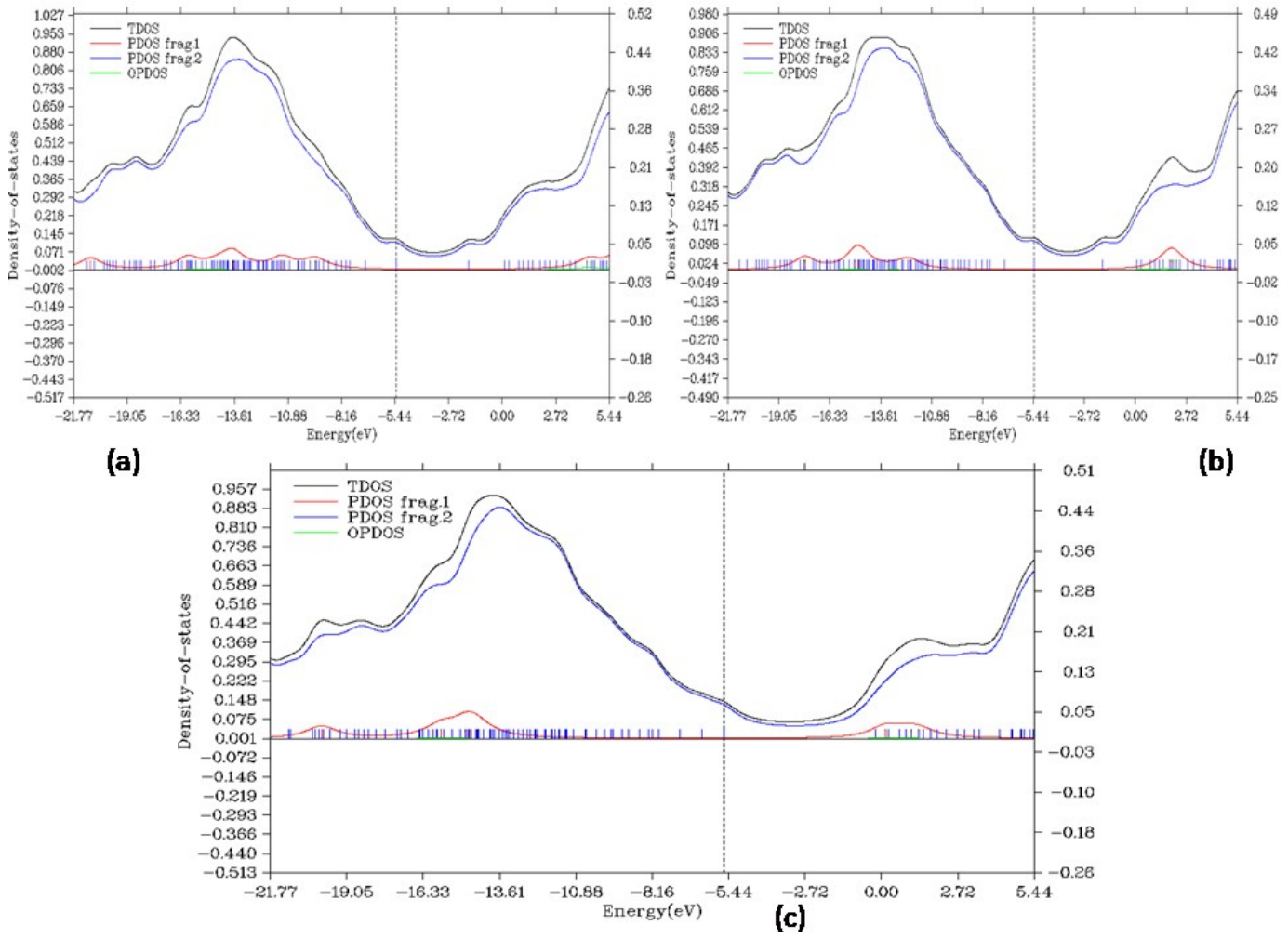

Figure S9. The TDOS plots of CO/NO/CH_3OH@BNGR where (a) CH_3OH@BNGR, (b) CO@BNGR and (c) NO@BNGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes BNGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

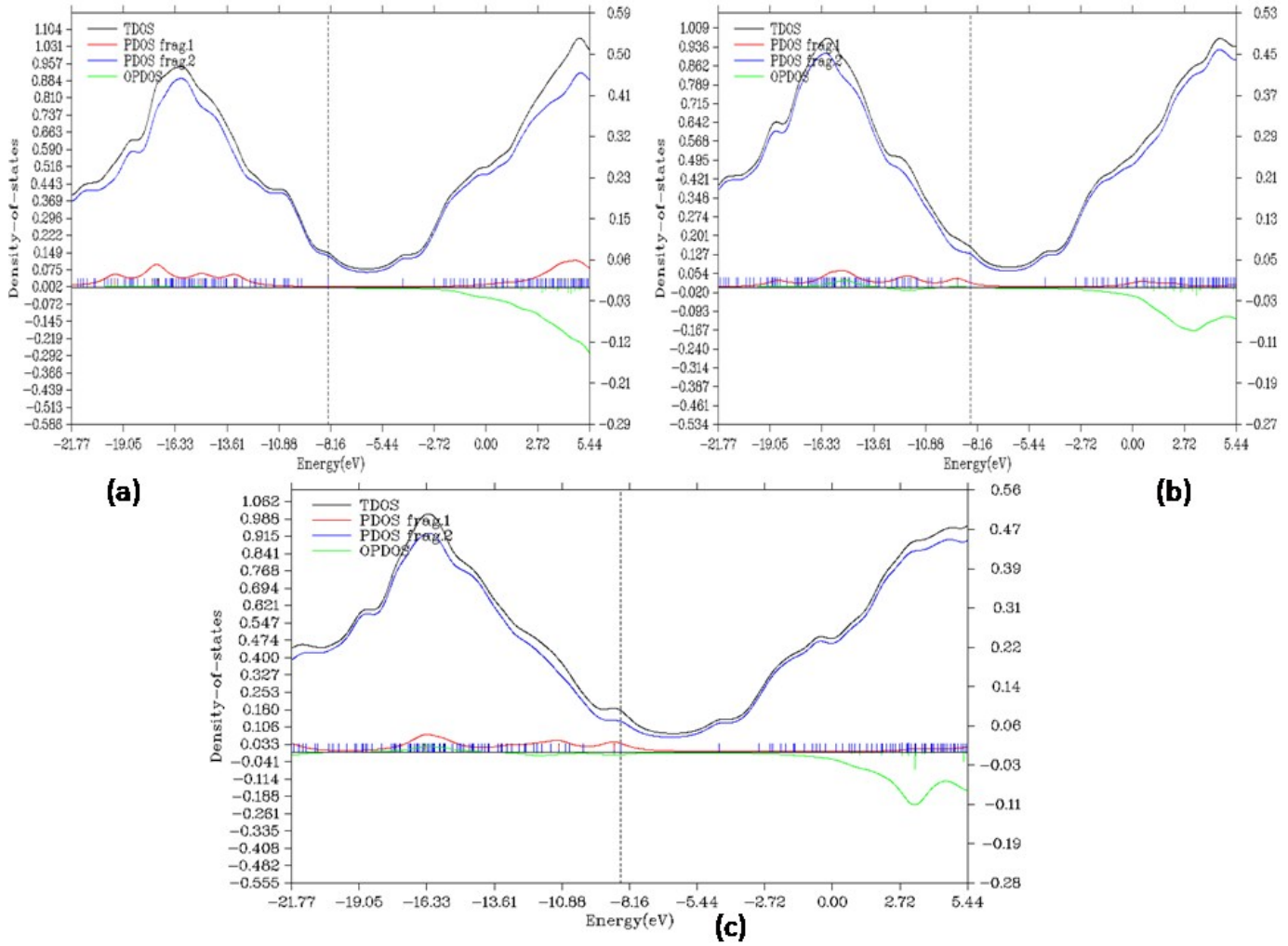

Figure S10. The TDOS plots of $CO/NO/CH_3OH@Li_3O^+GR$ where (a) $CH_3OH@Li_3O^+GR$, (b) $CO@Li_3O^+GR$ and (c) $NO@Li_3O^+GR$ respectively. Here frag1 denotes $CO/NO/CH_3OH$ moieties whereas frag2 denotes $Li_3O^+@GR$. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

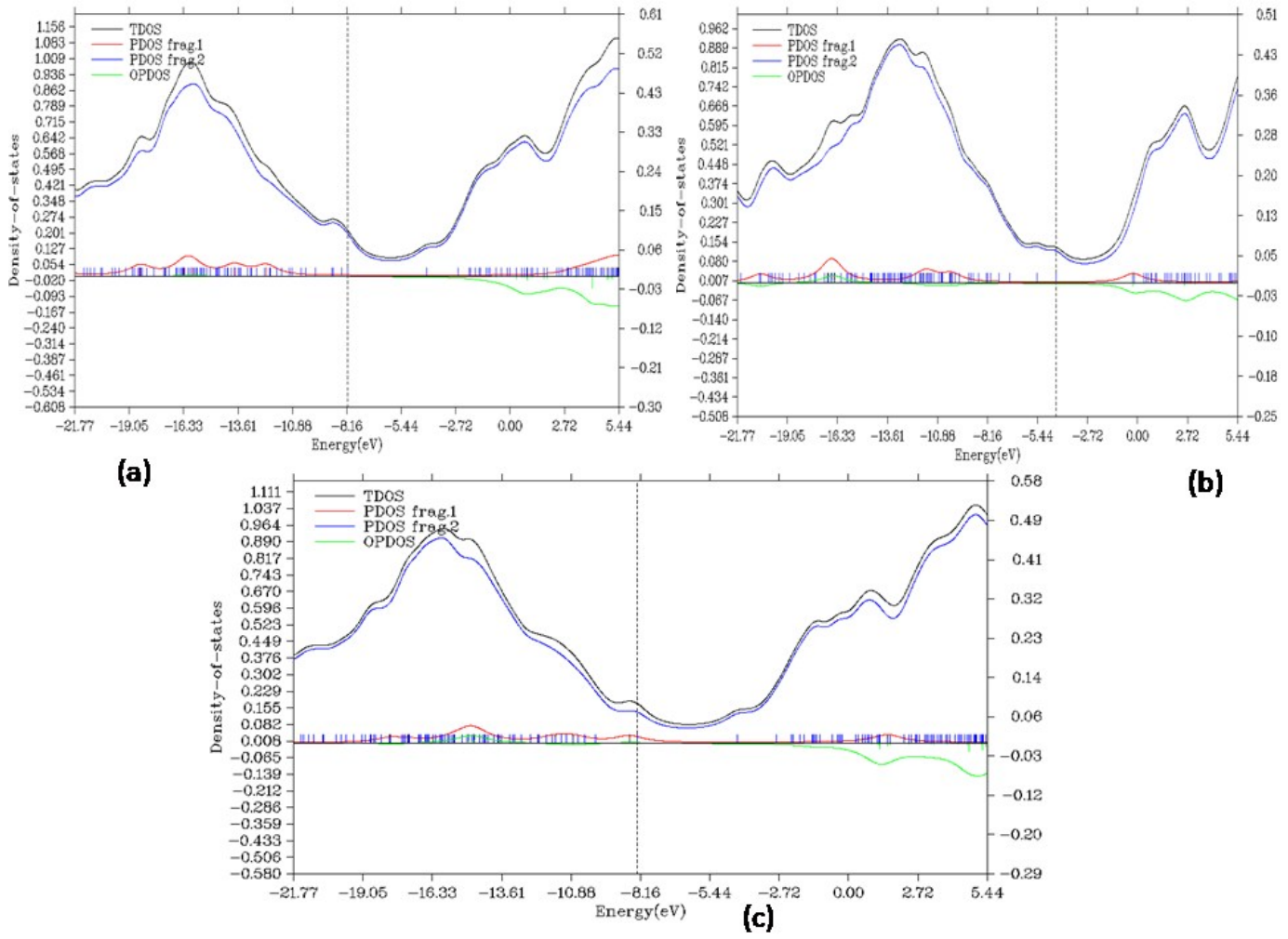

Figure S11. The TDOS plots of CO/NO/CH_3OH@Na_3O^+GR where (a) CH_3OH@ Na_3O^+GR, (b) CO@Na_3O^+GR and (c) NO@ Na_3O^+GR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes Na_3O^+@GR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

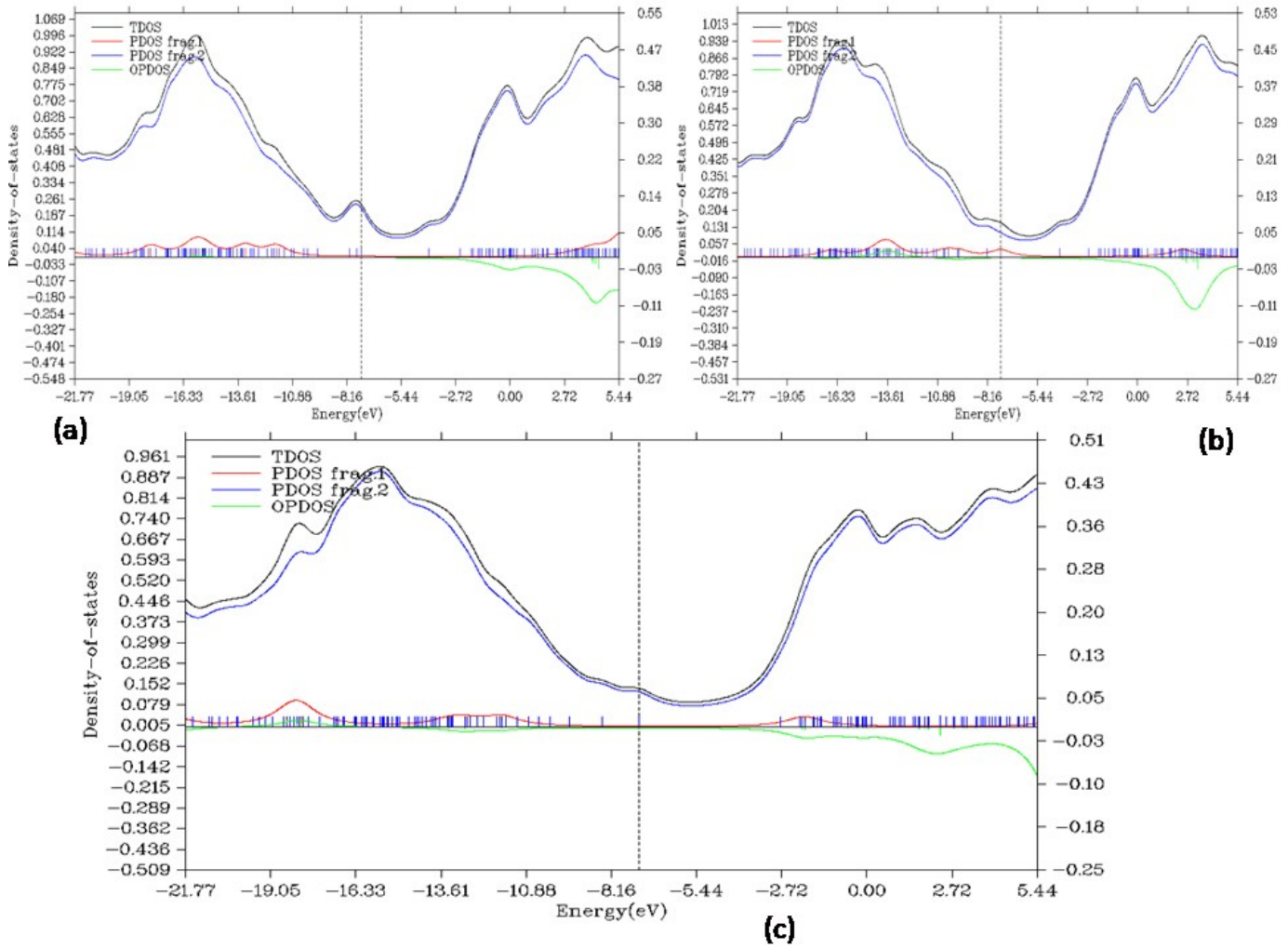

Figure S12. The TDOS plots of CO/NO/CH_3OH@K_3O^+GR where (a) CH_3OH@ K_3O^+GR, (b) CO@K_3O^+GR and (c) NO@K_3O^+GR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes K_3O^+@GR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

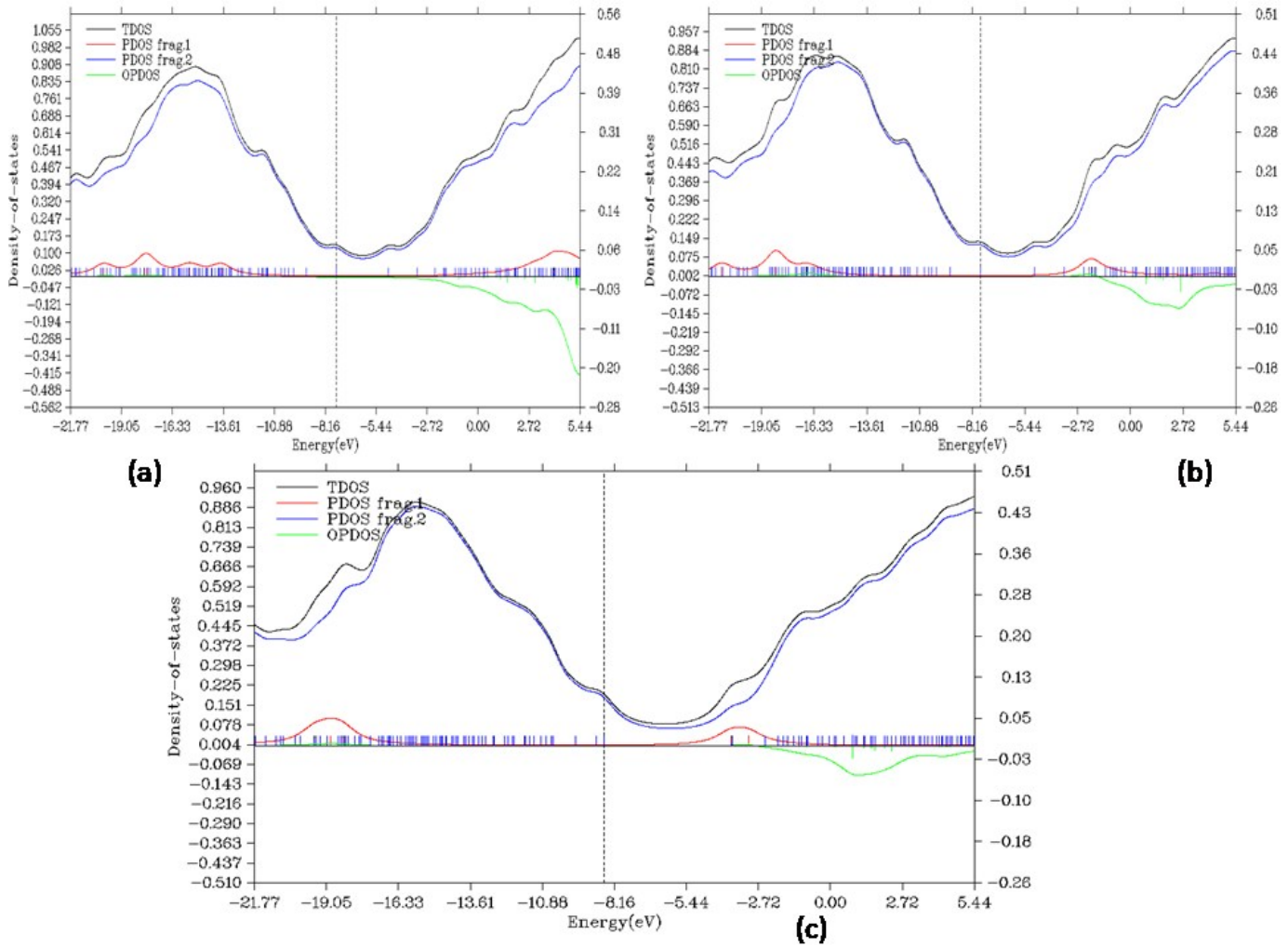

Figure S13. The TDOS plots of CO/NO/CH_3OH@Li_3O^+BGR where (a) CH_3OH@Li_3O^+BGR, (b) CO@Li_3O^+BGR and (c) NO@Li_3O^+BGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes Li_3O^+@BGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

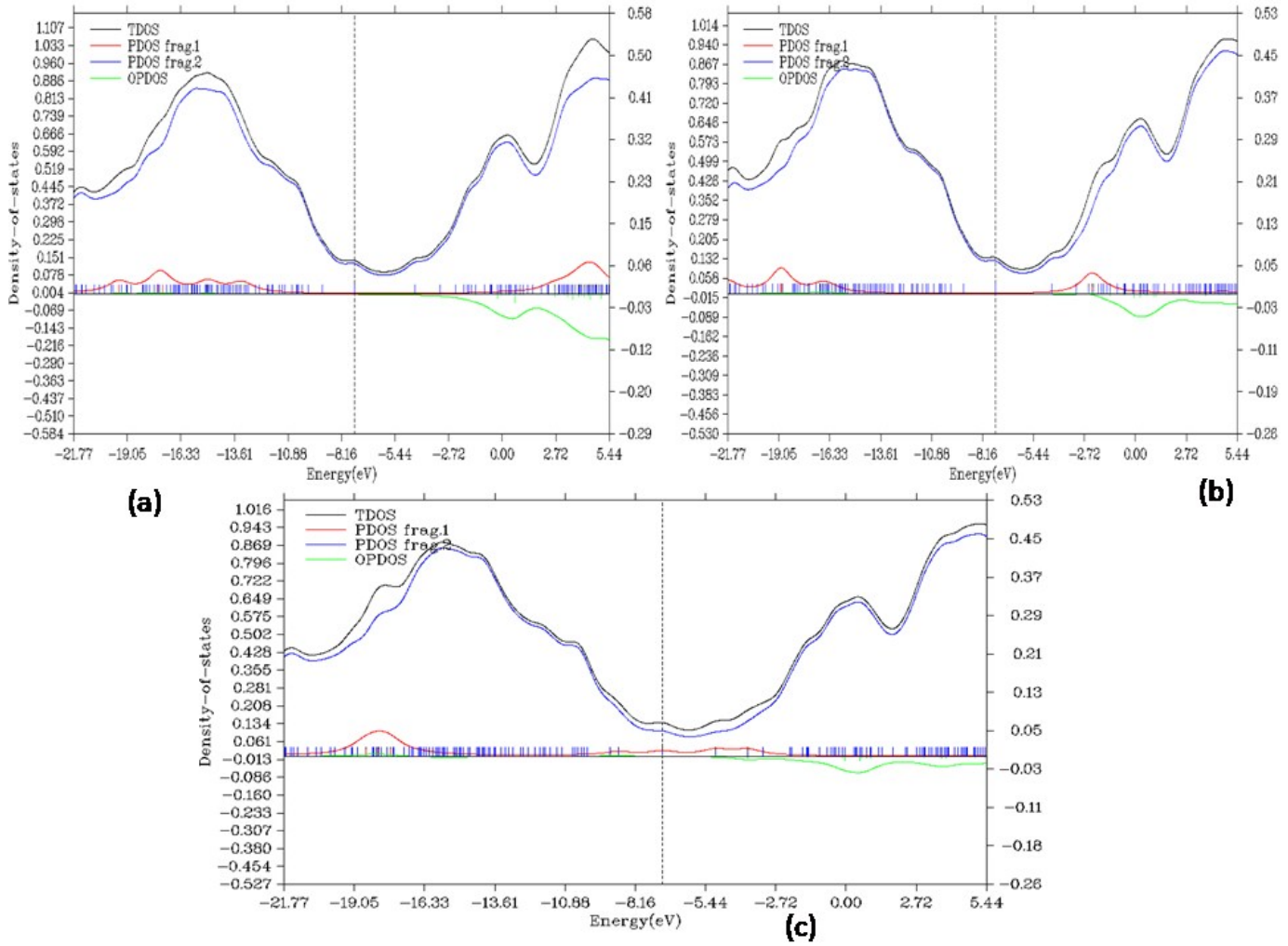

Figure S14. The TDOS plots of CO/NO/CH_3OH@Na_3O^+BGR where (a) CH_3OH@ Na_3O^+BGR, (b) CO@Na_3O^+BGR and (c) NO@Na_3O^+BGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes Na_3O^+@BGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

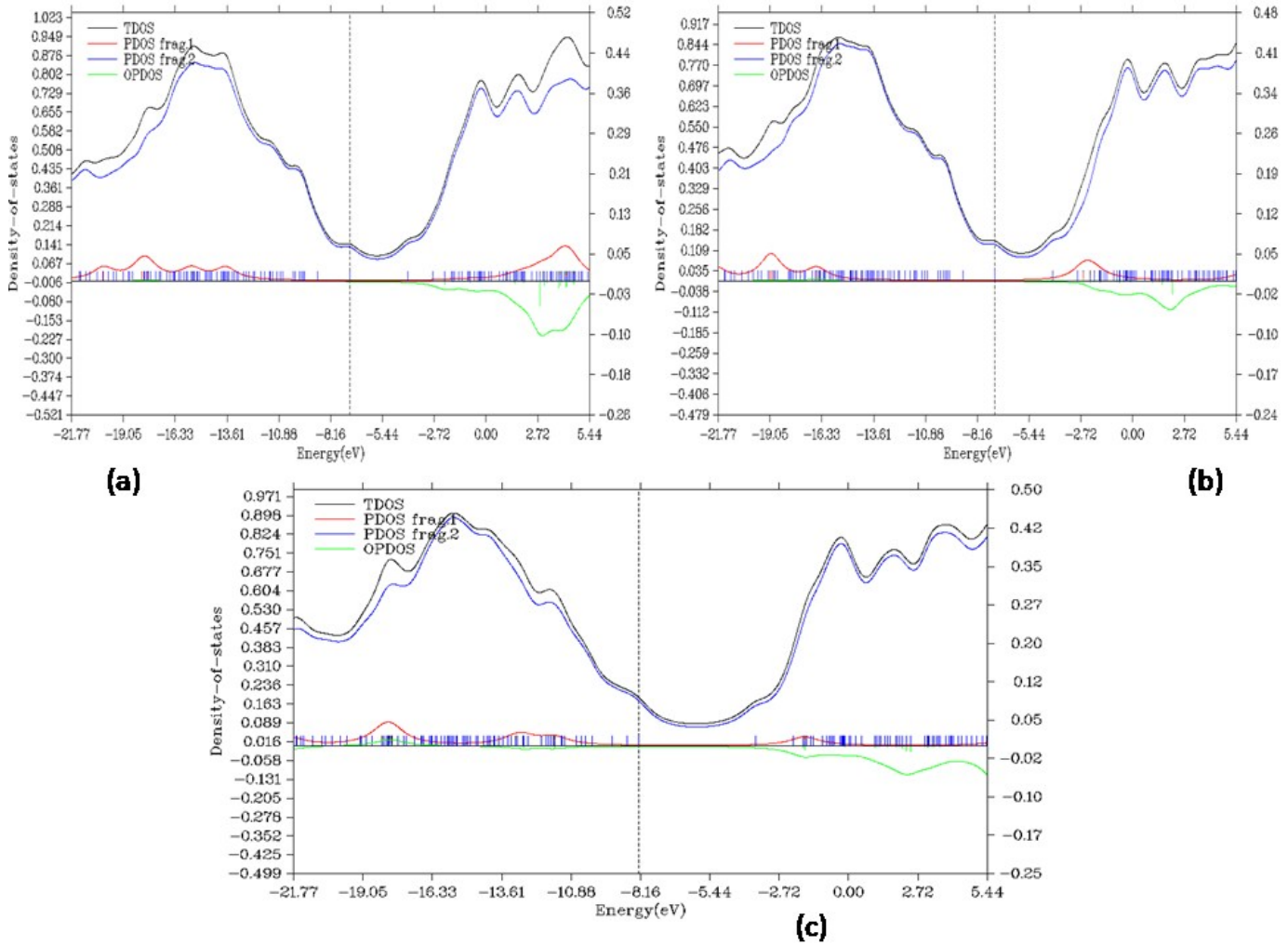

Figure S15. The TDOS plots of CO/NO/CH_3OH@K_3O^+BGR where (a) CH_3OH@ K_3O^+BGR, (b) CO@K_3O^+BGR and (c) NO@K_3O^+BGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes K_3O^+@BGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

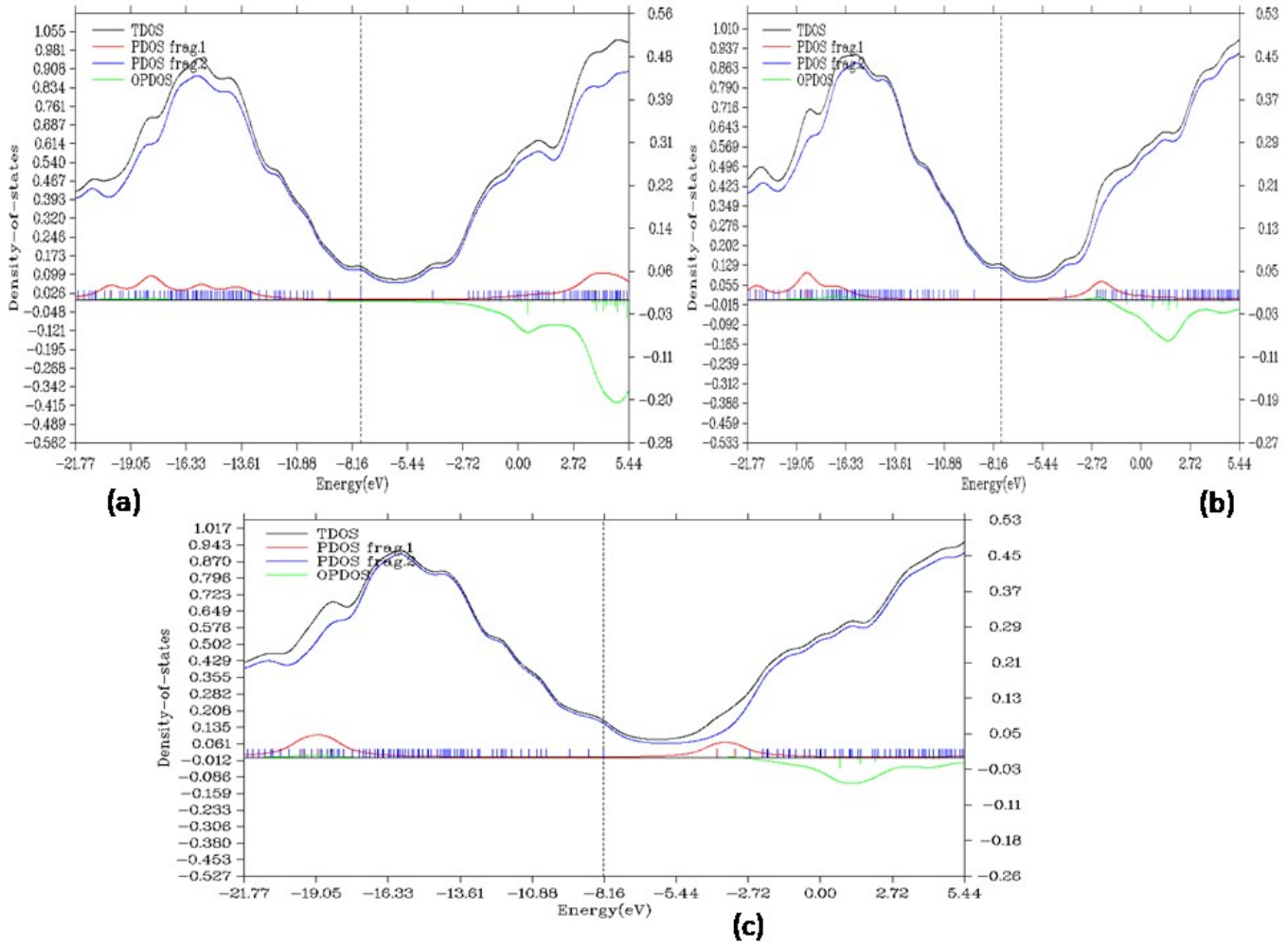

Figure S16. The TDOS plots of CO/NO/CH_3OH@Li_3O^+BNGR where (a) CH_3OH@Li_3O^+BNGR, (b) CO@Li_3O^+BNGR and (c) NO@Li_3O^+BNGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes Li_3O^+@BNGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

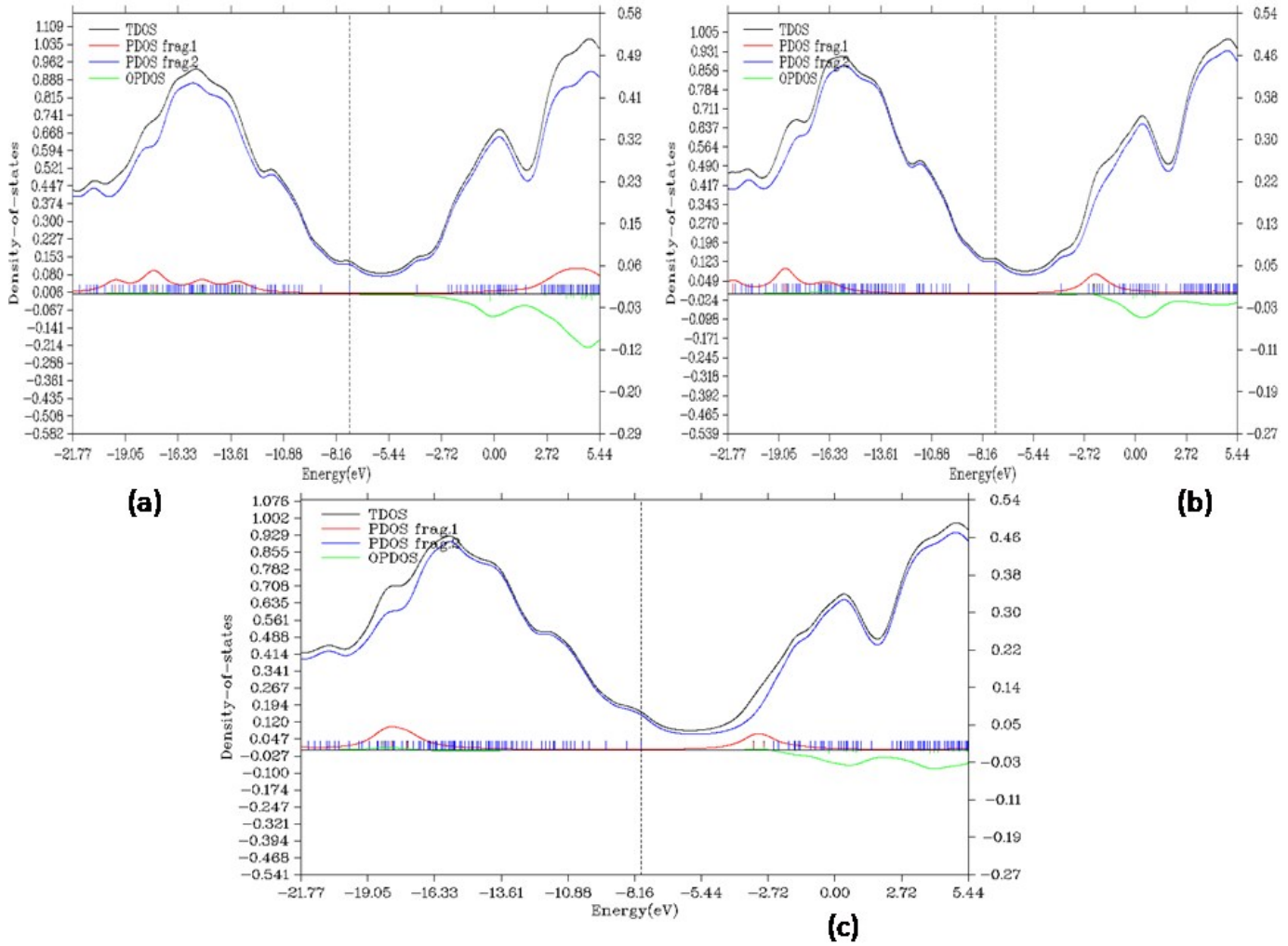

Figure S17. The TDOS plots of CO/NO/CH_3OH@Na_3O^+BNGR where (a) CH_3OH@ Na_3O^+BNGR, (b) CO@Na_3O^+BNGR and (c) NO@ Na_3O^+BNGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes Na_3O^+@BNGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.

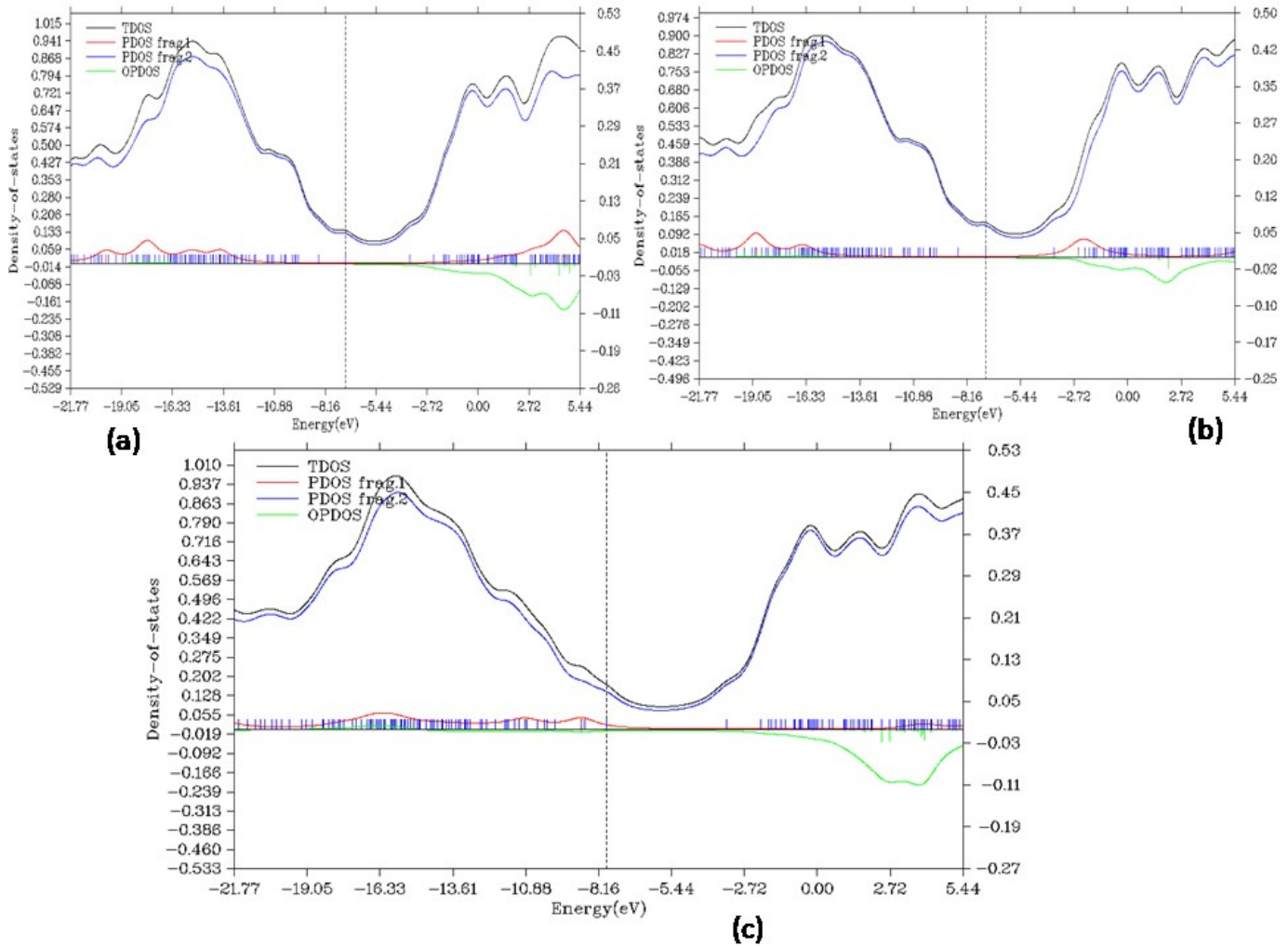

Figure S18. The TDOS plots of CO/NO/CH_3OH@K_3O^+BNGR where (a) CH_3OH@ K_3O^+BNGR, (b) CO@K_3O^+BNGR and (c) NO@K_3O^+BNGR respectively. Here frag1 denotes CO/NO/CH_3OH moieties whereas frag2 denotes K_3O^+@BNGR. The vertical line designates the E_F whereas the vertical bars represent occupied and virtual orbitals.