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

Supplementary information of the manuscript: Transition metal (Ti, Cu, Zn, Pt) single-atom modified graphene/AS_2 (A=Mo, W) van der Waals heterostructures for removing airborne pollutants

Erika Camarillo-Salazar[1], Reyes Garcia-Diaz[2], María Teresa Romero de la Cruz[3], Yuliana Avila-Alvarado[4], H. N. Fernandez-Escamilla[5], Gregorio Hernández Cocoletzi[6], J. Guerrero-Sanchez[7]

[1]Universidad Autónoma de Coahuila, Facultad de Ciencias Químicas, Boulevard Venustiano Carranza e Ing. José Cárdenas, 25280, Saltillo, Coahuila, México.
[2]CONACyT, Universidad Autónoma de Coahuila, Facultad de Ciencias Físico Matemáticas, Unidad Camporredondo, Edif. A, 25000, Saltillo, Coahuila, México.
[3]Universidad Autónoma de Coahuila, Facultad de Ciencias Físico Matemáticas, Unidad Camporredondo, Edif. A 25000, Saltillo, Coahuila, México.
[4]Universidad Autónoma de Coahuila, Facultad de Sistemas, Carretera a México Km 13, 25350 Arteaga, Saltillo, Coahuila, México.
[5]CICFIM Facultad de Ciencias Físico Matemáticas, Universidad Autónoma de Nuevo León, Nuevo Leon, 66450, San Nicolás de los Garza, México
[6]Benemérita Universidad Autónoma de Puebla, Instituto de Física "Ing. Luis Rivera Terrazas", Apartado Postal J-48, 72570, Puebla, Puebla, México.
[7]Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Apartado 5 Postal 14, 22800, Ensenada, Baja California, México.

Pollutant molecules adsorption on G/MoS_2 and G/WS_2

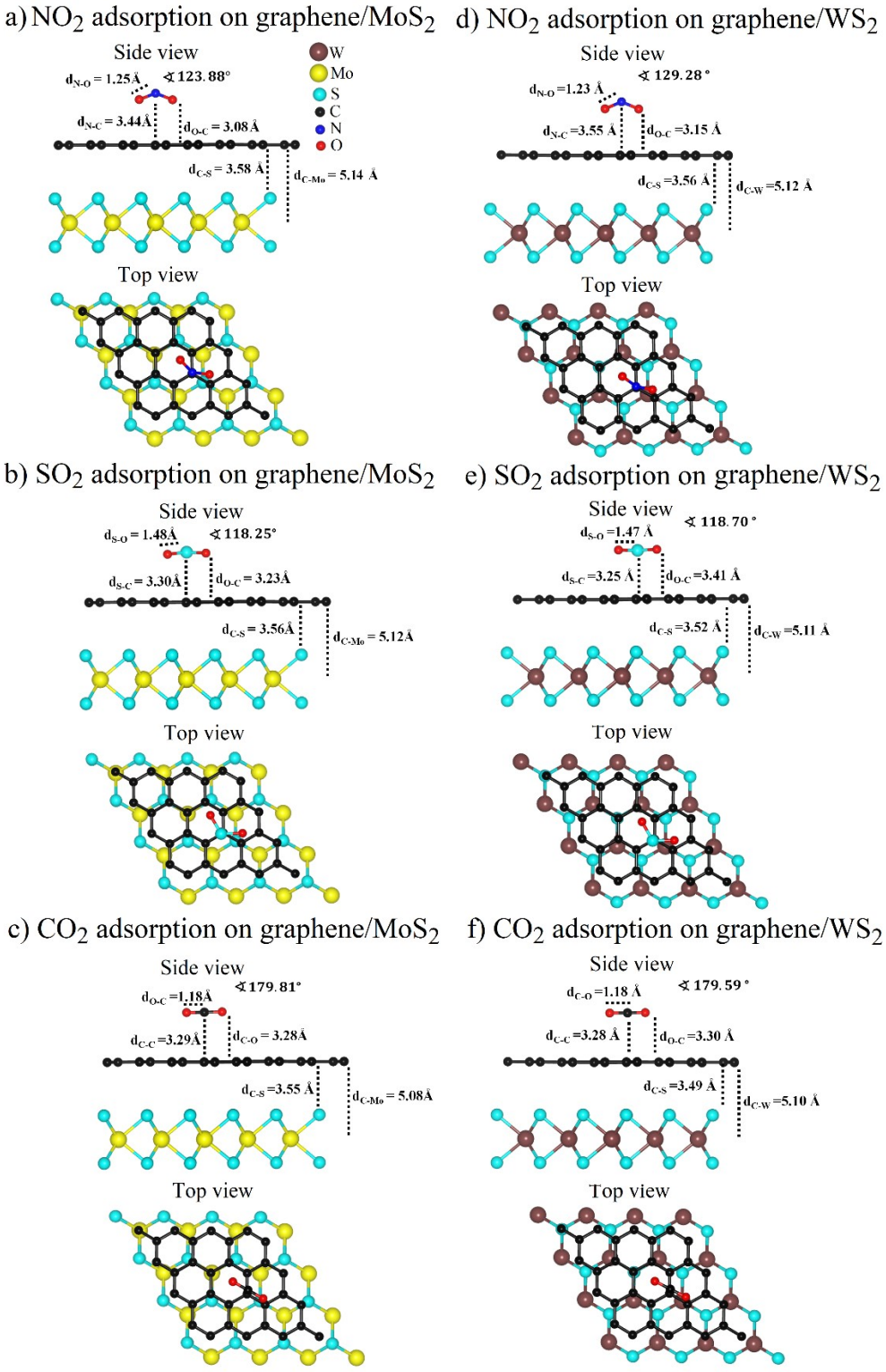

Fig. S1. Adsorption of NO_2, b) SO_2 and c) CO_2 molecules on (a) G/MoS_2 heterostructure and (b) G/WS_2 heterostructure, top and side views.

Transition metal single-atom G/MoS_2 and G/WS_2

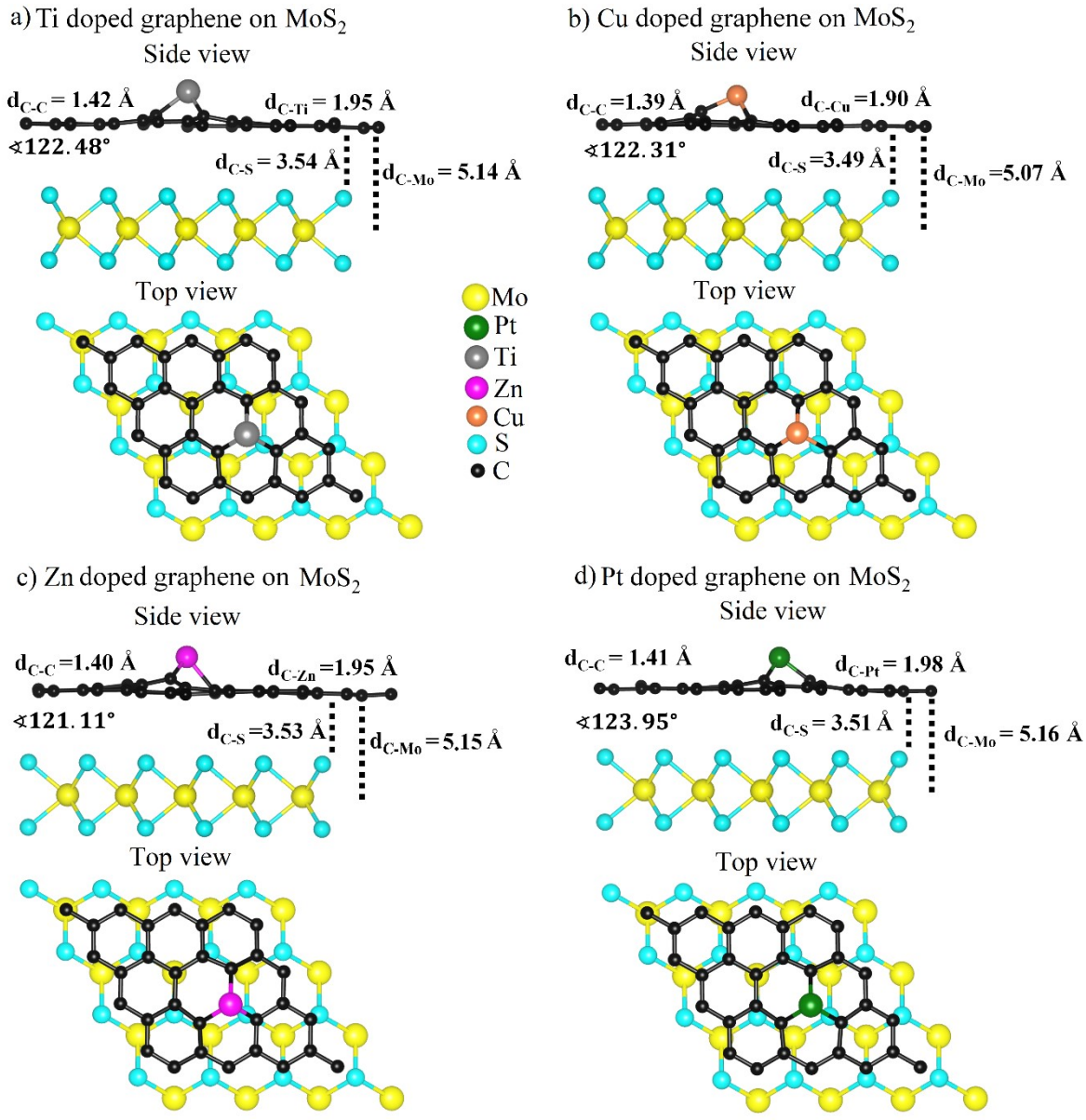

Fig. S2. Single-atom graphene, a) Ti, b) Cu, c) Zn, and d) Pt on MoS_2 heterostructure, top and side views.

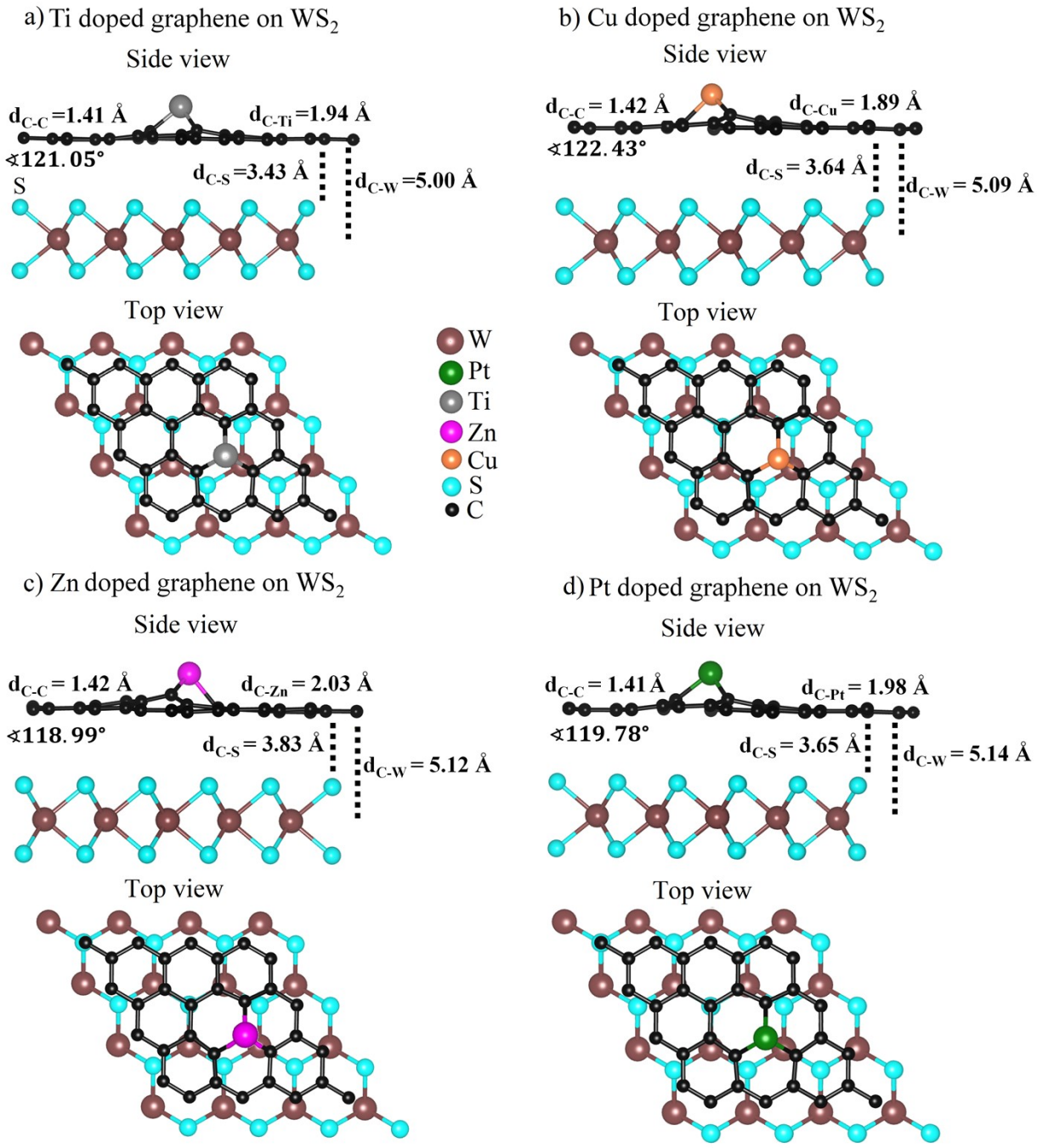

Fig. S3. Graphene doped with: a) Ti, b) Cu, c) Zn, and d) Pt on WS_2 heterostructure, top and side views.

Pollutant molecules adsorption on GSAC/MoS_2 and GSAC/WS_2

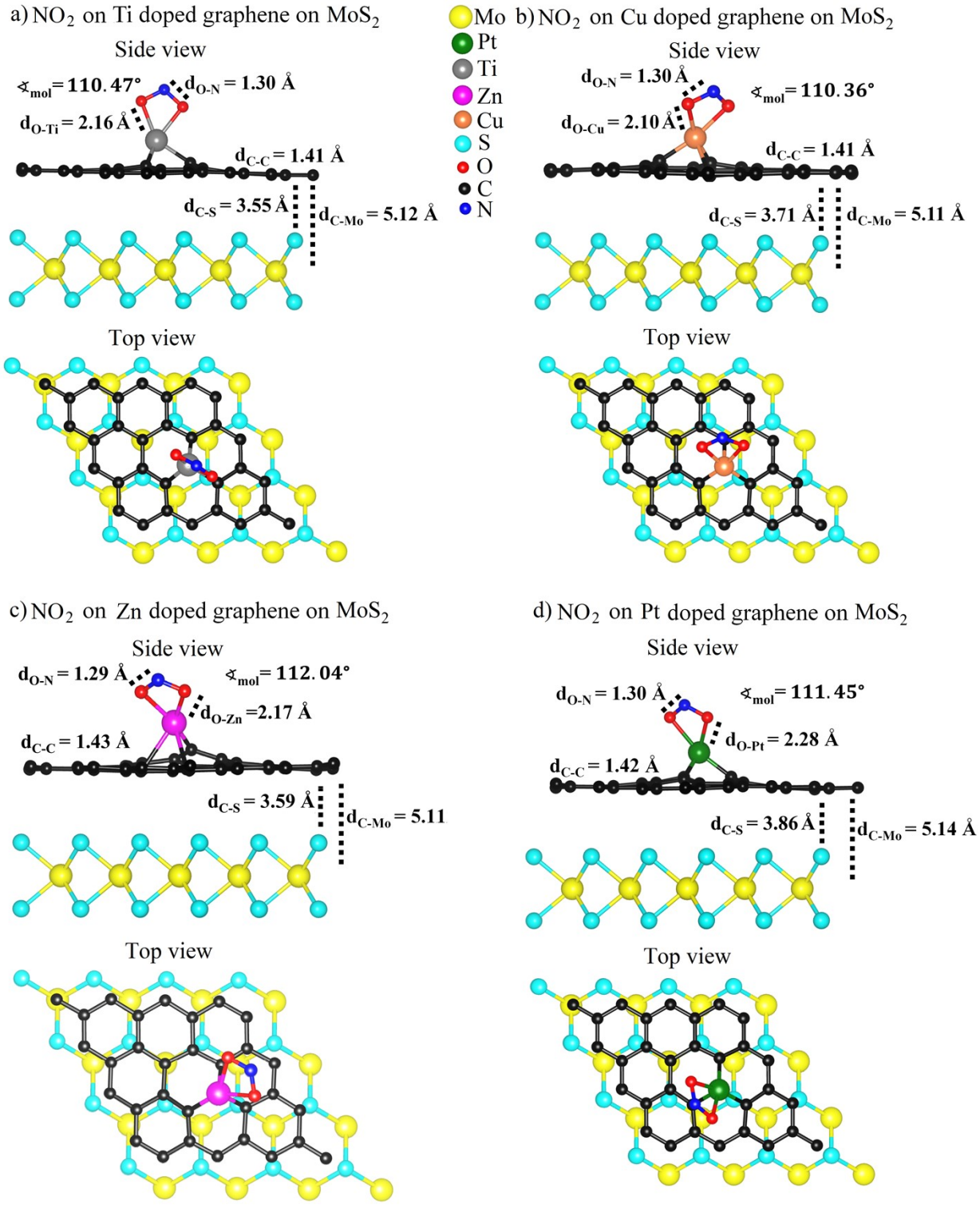

Fig. S4. Adsorption of NO_2 molecule on GSAC with a) Ti, b) Cu, c) Zn, and d) Pt on MoS_2 heterostructure, top and side views.

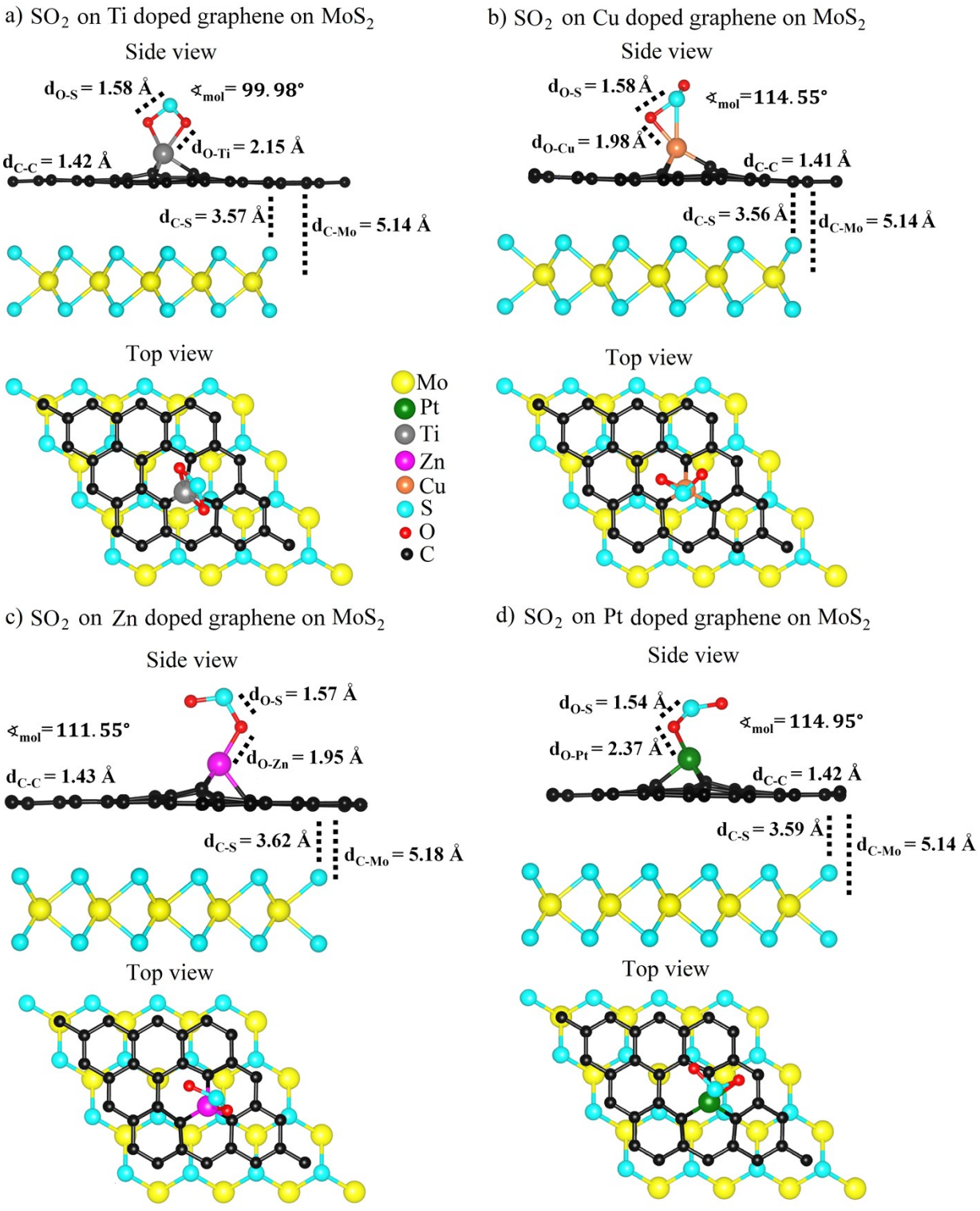

Fig. S5. Adsorption of SO_2 molecule on GSAC with: a) Ti, b) Cu, c) Zn, and d) Pt on MoS_2 heterostructure, top and side views.

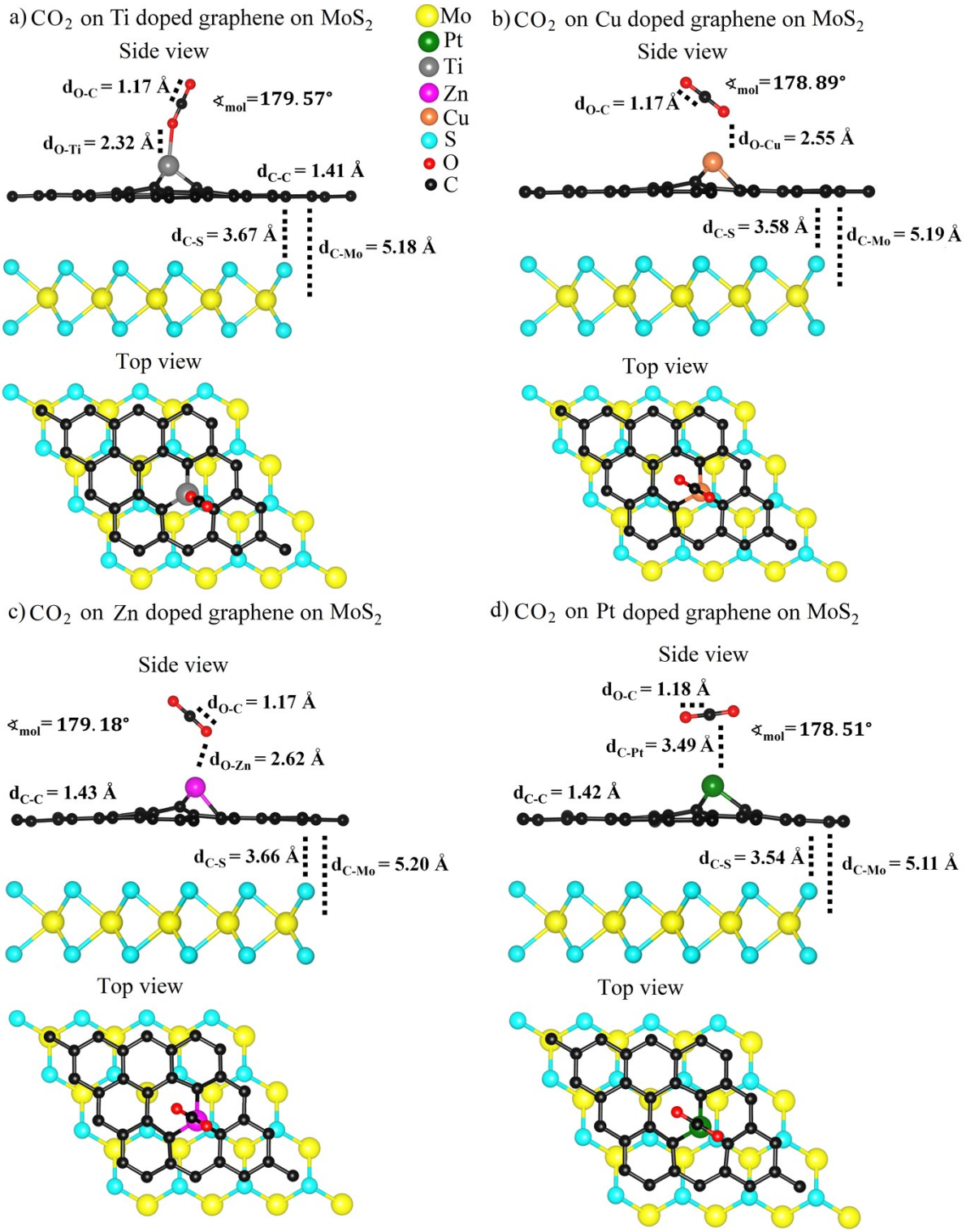

Fig. S6. Adsorption of CO_2 molecules on GSAC with: a) Ti, b) Cu, c) Zn, and d) Pt on MoS_2 heterostructure, top and side views.

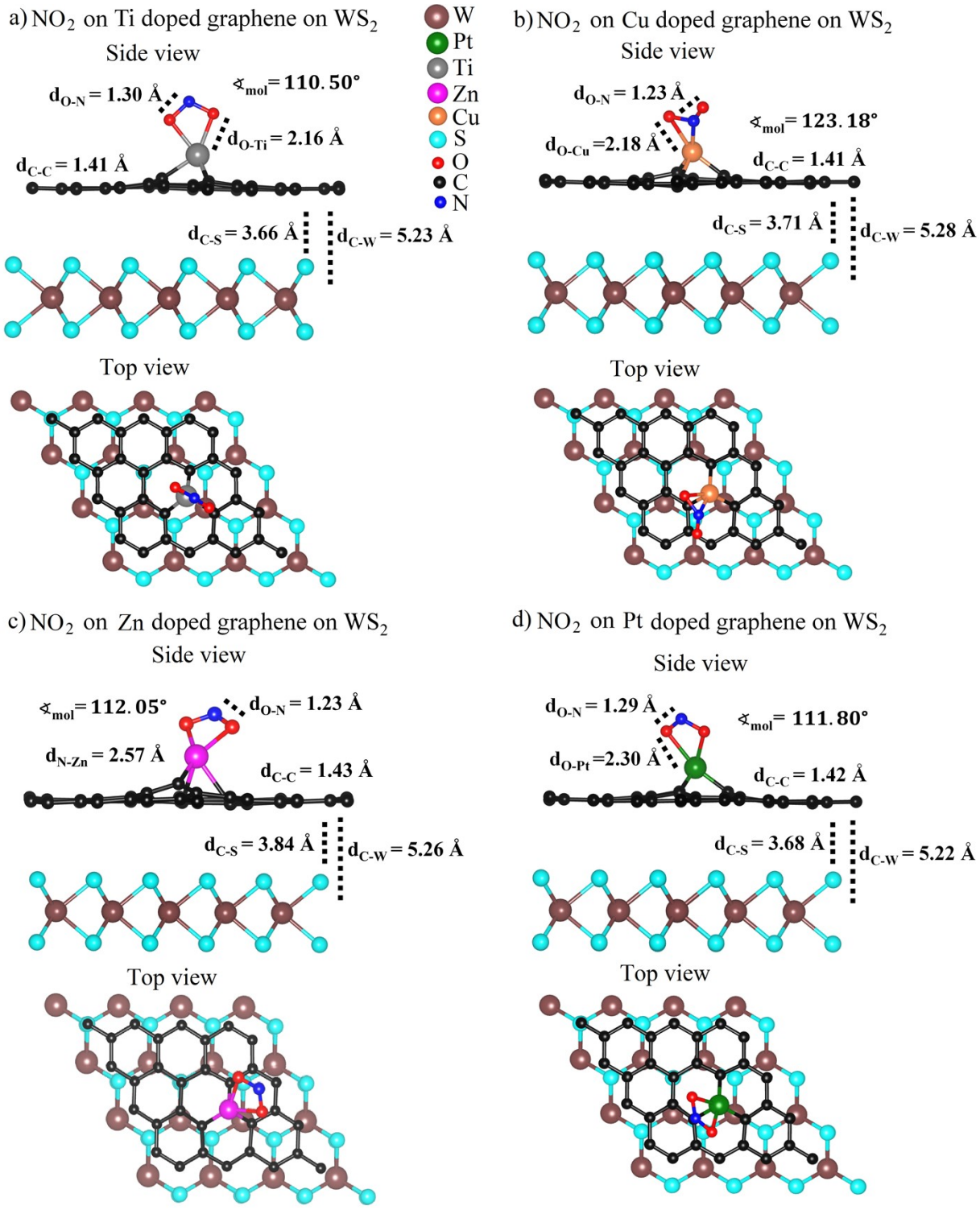

Fig. S7. Adsorption of NO_2 molecule on GSAC with: a) Ti, b) Cu, c) Zn, and d) Pt on WS_2 heterostructure, top and side views.

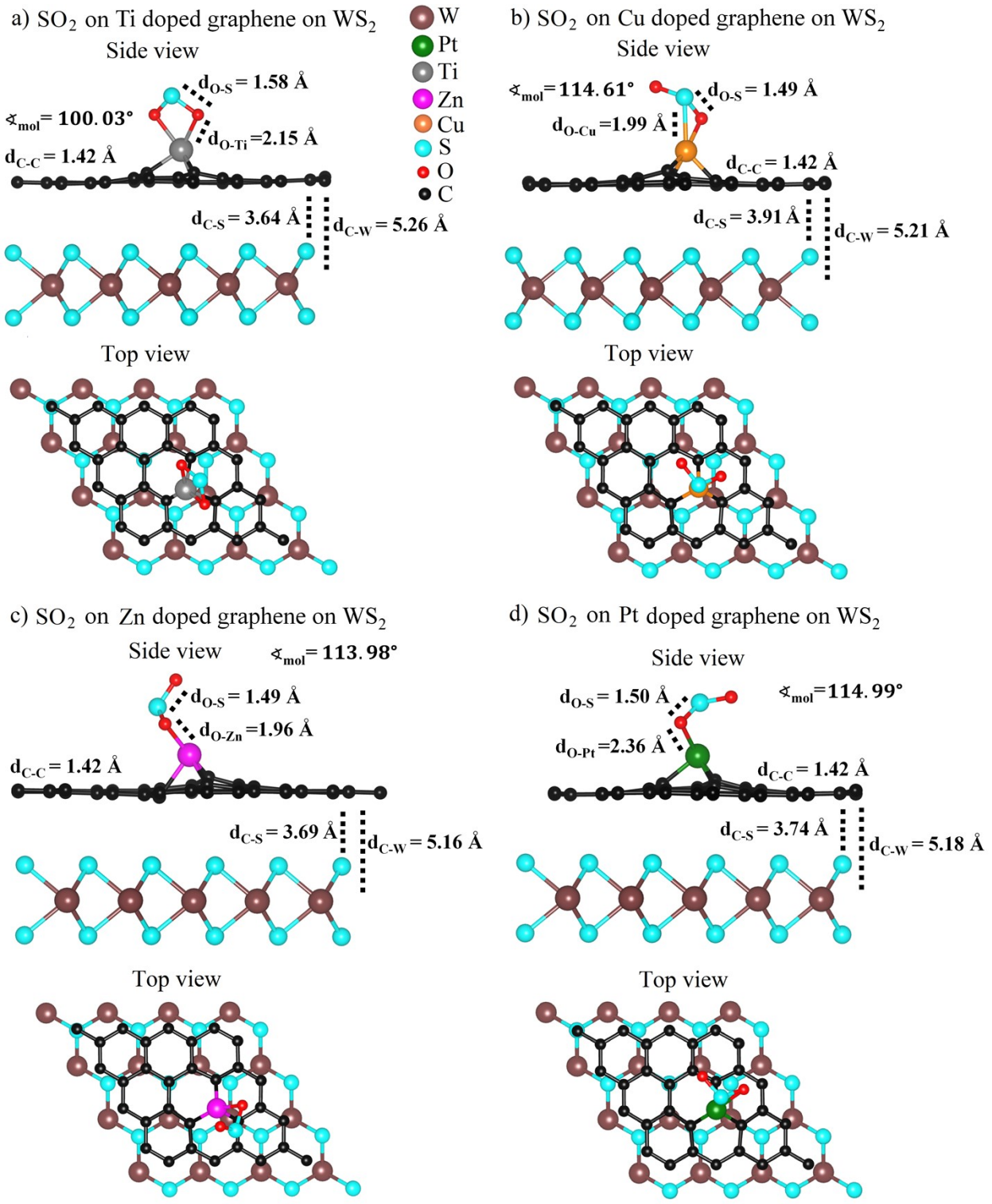

Fig. S8. Adsorption of SO_2 molecule on GSAC with: a) Ti, b) Cu, c) Zn, and d) Pt on WS_2 heterostructure, top and side views.

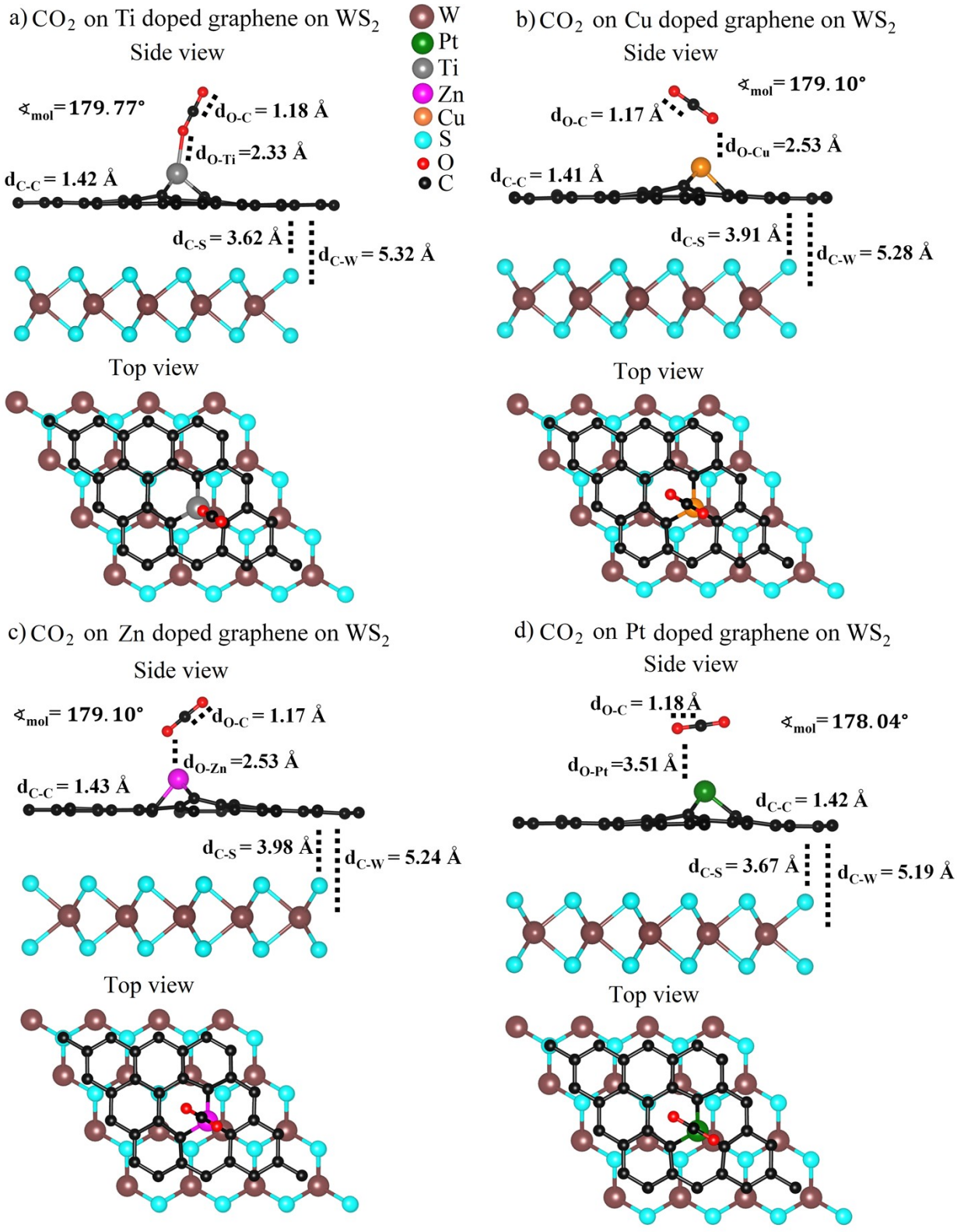

Fig. S9. Adsorption of CO_2 molecule on GSAC with a) Ti, b) Cu, c) Zn, and d) Pt on WS_2 heterostructure, top and side views.

Table 1S. Adsorption energy, E_{ads}, per supercell.

	Adsorption energy (eV/supercell)
$NO_2/G/MoS_2$	-0.32
$NO_2/G/WS_2$	-0.31
$NO_2/G:Ti/MoS_2$	-3.11
$NO_2/G:Ti/WS_2$	-2.92
$NO_2/G:Cu/MoS_2$	-2.61
$NO_2/G:Cu/WS_2$	-2.22
$NO_2/G:Zn/MoS_2$	-2.31
$NO_2/G:Zn/WS_2$	-2.36
$NO_2/G:Pt/MoS_2$	-2.32
$NO_2/G:Pt/WS_2$	-2.36
$SO_2/G/MoS_2$	-0.30
$SO_2/G/WS_2$	-0.30
$SO_2/G:Ti/MoS_2$	-1.64
$SO_2/G:Ti/WS_2$	-1.64
$SO_2/G:Cu/MoS_2$	-1.09
$SO_2/G:Cu/WS_2$	-1.19
$SO_2/G:Zn/MoS_2$	-0.91
$SO_2/G:Zn/WS_2$	-1.74
$SO_2/G:Pt/MoS_2$	-1.00
$SO_2/G:Pt/WS_2$	-1.01
$CO_2/G/MoS_2$	-0.20
$CO_2/G/WS_2$	-0.19

CO_2/G:Ti/MoS_2	-0.46
CO_2/G:Ti/WS_2	-0.47
CO_2/G:Cu/MoS_2	-0.10
CO_2/G:Cu/WS_2	-0.17
CO_2/G:Zn/MoS_2	-0.13
CO_2/G:Zn/WS_2	-0.27
CO_2/G:Pt/MoS_2	-0.09
CO_2/G:Pt/WS_2	-0.09