

Supplementary Documents:

Figure S1: Device of functionalized MoS₂: (a) before adsorption, (b) after adsorption of NO molecule, and (c) after adsorption of NO₂ molecule. (d) TDOS due to MoS₂ NR in pristine and (V_S, Mn, Fe, Co, and Ni)-functionalized forms.

Figure S2: Differential resistance versus bias due to the adsorptions of NO and NO₂ gas molecules on five samples: (a) MoS₂:V_S, (b) MoS₂:Mn, (c) MoS₂:Fe, (d) MoS₂:Co, and (e) MoS₂:Ni.

Figure S3: Sensor response versus bias due to the adsorptions of NO and NO₂ gas molecules on five samples: (a) MoS₂:V_S, (b) MoS₂:Mn, (c) MoS₂:Fe, (d) MoS₂:Co, and (e) MoS₂:Ni.

Figure S4: The initial and final configurations of relaxing two molecules (NO and N₂), simultaneously, on MoS₂:Ni@S surface. NO molecule favors chemisorption on Ni dopant while N₂ molecule remains in a physisorption state. Color of atoms: Mo (cyan), S (yellow), Ni (green), N (blue), O (red).