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

Electronic Supplementary Information (ESI)

Highly infrared sensitive VO_2 nanowire as nano-optical device

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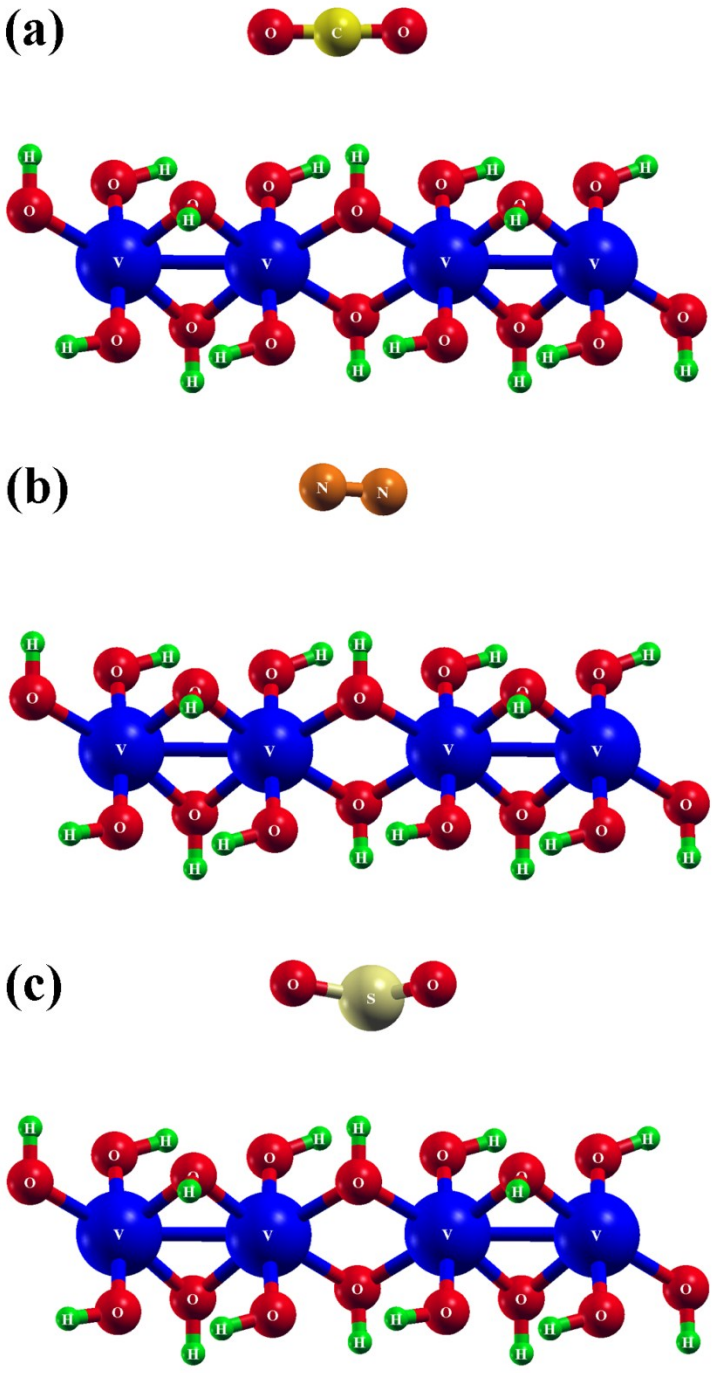

Figure S1: The optimized monoclinic structure of (a) CO_2 gas molecule adsorbed on 1D VO_2, (b) N_2 gas molecule adsorbed on VO_2 nanowire and (c) SO_2 gas molecule adsorbed on VO_2 nanowire structure.

Table S1: Structural parameters of 1D VO_2 rutile and monoclinic structure nanowires calculated within GGA and GGA+U method. The experimental values [18] of V-V bond length of bulk VO_2 is also given for comparison.

Structure	Lattice constant, a (Å)	V-V bond length for VO_2 NW(Å)	V-V bond length in bulk VO_2		
			GGA	GGA+U	Expt [1]
VO_2(R)	5.70	2.86	3.01	2.81	2.85
VO_2(M)	5.73	2.60	2.47	2.56	2.66
		3.13	3.12	3.16	3.12

Table S2: Table for polarization and magnetic moment for VO_2(R) and VO_2(M)

Structure	Polarization	Magnetic moment (Bohr magneton)
VO_2(M)	0	0.30
VO_2(R)	1	0.41

Table S3: Different parameters like bond length (b) of gas molecules, bond angle (θ), change in bond length (Δb), change in bond angle (Δθ), change in charge transfer (ΔQ) and adsorption energy (E_{ad}) of different gas molecules adsorbed on monoclinic VO_2 nanowire structure.

	Free molecules		Adsorption of gas molecules on VO_2(M) nanowire			
Gas Molecules	**b (Å)**	**θ (º)**	**Δb (Å)**	**Δθ (º)**	**ΔQ**	**E_{ad} (eV)**
SO_2	1.47	119	0.01	0.7	0.4877	-0.30
N_2	1.10	-	0.01	-	0.1582	-0.06
CO_2	1.16	180	0.01	0.84	0.2721	-0.12

References

1. J. Zhang, H. He, Y. Xie and B. J. Pan, Chem. Phys., 2013, **138(11)**, 114705.