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Highly infrared sensitive VO_2 nanowire as nano-optical device

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Recent studies on electronic, magnetic and optical properties of VO_2 (vanadium dioxide) material motivates to explore one dimensional VO_2 nanowires. First principles calculations are performed to investigate structural, electronic, magnetic and optical properties of monoclinic (M) and rutile (R) phase of VO_2 nanowire. The monoclinic phase shows semiconducting behaviour with a band gap of 1.17eV; whereas the rutile phase of VO_2 nanowire behaves as spin gapless semiconducting material, as band lines cross the Fermi level due only up spin contribution. The monoclinic structure of VO_2 nanowire is found to be paramagnetic, while the rutile structure is ferromagnetic half metal. Our conductivity calculation for VO_2 nanowire shows metal-insulator transition temperature to be 250K. The possible mechanism of VO_2 nanowire to be used as smart windows has been discussed, as the nanowire is highly sensitive in the infrared (IR) region. Interestingly, at low temperature, VO_2 monoclinic structure allows infrared light to transmit while VO_2 with rutile phase block light in the IR region. Furthermore, we adsorbed CO_2, N_2 and SO_2 gas molecules on 1D VO_2 monoclinic nanowire to investigate their interaction behaviour. It has been observed that absorption and transmission properties of VO_2 show dramatic change on the adsorption of CO_2 and SO_2 gas molecules, which is likely to open up its application as optical gas sensor.

Introduction

Vanadium oxide (VO_2) undergoes reversible metal-insulator phase transition at 341K from monoclinic zigzag VO_2(M) structure to tetragonal rutile VO_2(R) structure [1, 2]. The geometrical deformation of VO_2 results into the change in electrical resistivity at transition temperature, thereby, shows an ability to convert thermal energy to electrical energy. Therefore, VO_2 is a promising thermoelectric material for energy harvesting [3, 4]. Furthermore, structural deformation driven transition causes change in the magnetization and optical reflectivity of VO_2, e.g., an abrupt change in infrared transmittance at transition temperature (T_c) [5] makes it a promising material for optical energy devices, optical sensors and 'smart windows' [6-9]. The change in magnetization due to phase transition is a good sign for VO_2 to be useful for magnetic refrigeration which is based on magneto caloric effect (MCE) [10].

In the past few decades, VO_2 has been studied to analyse the mechanism behind its phase transition. It has been debated for long time, whether the transition is due to Mott model which is based on electronic correlation, or electron-phonon correlation based Peierls Model, or the both. The clear picture for the phase transition behaviour is till now undisputed [11, 12]. However, the T_c is very high for practical usage. Previous theoretical and experimental studies have shown that T_c can be lowered by doping with foreign impurities, e.g., tungsten dopant lowers Tc upto 257K, while Zr-doping shows phase transition at 337.3K [13-20]. The MIT behaviour in VO_2 NW can be tuned to lower temperature by appropriate doping [21] or by axial stress [22, 23]. For example, ion diffusion in single crystalline VO_2 nanowire using ionic liquid (IL) gating has been described by change in the charge carrier concentration associated with ion doping [24]. Moreover VO_2 is one of the most promising candidates for battery industries and energy storage devices [25- 29].

In the last few years, one-dimensional (1D) nanowires have gained immense interest due to their unique electronic, magnetic, mechanical, optical properties. High surface area and very high density of electronic states at Fermi energy region of nanowire enhanced exciton binding energy and increased surface scattering for electron and phonon. This attributed to nanowires having different properties from their corresponding bulk materials. In this regard, VO_2-NW has also been studied extensively [30, 31]. Wu, X. et al. [32] reported the synthesis of VO_2 nanowire and experimentally confirmed its transition temperature to be around 341K. Furthermore, Naoi, Y.et al. [5] investigated the size of the VO_2 nanowire for transmittance efficiency. It has been reported that 1D VO_2¬ nanowire having diameter of 50nm and length of 100nm provide better luminescence and thermochromic properties. Li, Z. et al. [33] studied the hydrogen effect on VO_2 nanowire to regulate the spin structure. VO_2 nanowires have shown potential application for the developments of ultrasensitive

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transition edge sensors (TES) for gas sensing. Note that the conductance of the nanowire essentially changes with the molecular composition, pressure and temperature of the ambient gas environment at transition edges [9]. Recently, Strelcov, E. et al. [9] has shown VO_2 to be a potential material as transition edge sensors for gas sensing.

VO_2 material showing such interesting properties at transition temperature like MIT behaviour, abrupt change in infrared transmittance, and recent research on VO_2 NW motivated us to study its change in the properties due to geometrical deformation with respect to change in temperature. In this context, we have considered rutile and monoclinic phase of 1D VO_2 nanowire. The objective of this paper is to provide better understanding of the influence of structural distortion on electronic structure using GGA+U method. The importance of optical and magnetic properties of both the structures has also been highlighted. Next, we consider the adsorption of CO_2, N_2 and SO_2 gas molecules on VO_2(M) nanowire to study the electronic and optical properties.

Computational Details

Theoretical calculations were performed using Quantum espresso package based on density functional theory (DFT) [34, 35]. The exchange correlation functional was treated within generalized gradient approximation (GGA) using Perdew-Burke-Ernzerof (PBE) functional. The on-site coulomb interactions are described by Hubbard U parameter which was set to be 3.4 eV [36, 37] in our calculations. The kinetic energy cut-off for the plane wave was taken 100 eV. We used a grid of 20×1×1 of k-points for Brillouin zone sampling with Monkhorst–Pack scheme [38]. The VO_2 structures were relaxed until the force on each atom was smaller than 0.01eV/Å. We used vacuum of 16Å along b- and c-axis to avoid any kind of interactions due to periodic images. To study the optical properties for VO_2 nanowire, random phase approximation (RPA) method together with DFT was used. The frequency dependent complex dielectric function $\varepsilon(\omega)$ can be written as $\varepsilon(\omega)= \varepsilon_1(\omega)+ i\varepsilon_2(\omega)$. Here, $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary part of complex dielectric function, respectively. The imaginary part is obtained from the summation over electronic states and is related to the absorption spectra. The real part of dielectric function, absorption and transmission spectra is determined from the Kramers-Kronig (KK) relation. Due to anisotropic behaviour of VO_2, we have considered the imaginary and real parts of dielectric function corresponding to electric field vectors parallel and perpendicular to the V-V chains to analyse absorption, transmittance and refractive index for VO_2 nanowire [39-43].

Results and discussions

Structural properties VO_2 NW

We have firstly relaxed tetragonal rutile, VO_2(R), and monoclinic zigzag VO_2 (M) bulk structure by both GGA and GGA+U method. We found that V-V bond length of bulk structure calculated with GGA+U method has close agreement with the experimental values (Table S1). Zhang, J. et al. [18] calculated V-V bond length for bulk VO_2 structure and reported V-V bond length of 2.837 Å for VO_2(R) and, 3.190 Å and 2.440 Å for VO_2(M). The both considered bulk structures are confined in y- and z-direction to have VO_2 NWs. The surfaces of the both nanowires are passivated with hydrogen atoms, so that all O atoms are sp-coordinated to prevent daggling bonds. The rutile structure, VO_2 (R), contains a V-V linear chain, where all V-atoms are arranged uniformly as shown in Figure 1. The diameters of our considered nanowires are 3.00Å for rutile structure and 3.98Å for monoclinic structure.

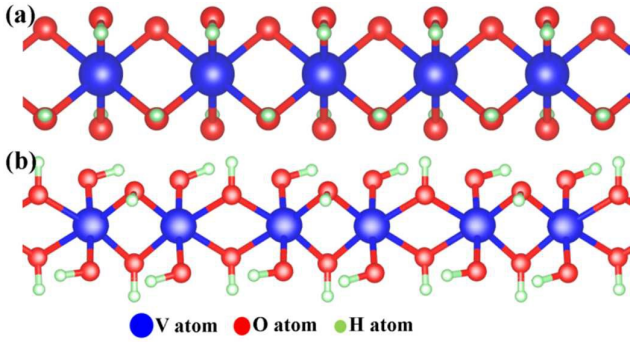

Figure 1: The optimized rutile and monoclinic structure of 1D VO_2. (a) Front view of rutile VO_2 structure. (b) Front view of monoclinic VO_2 structure.

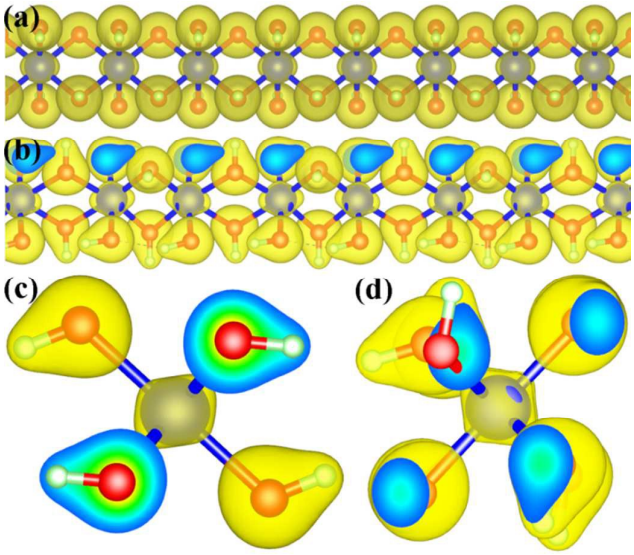

Figure 2: The calculated electronic charge density for 1D VO_2 rutile structure and 1D VO_2 monoclinic structure. (a) Top view of distribution of charge for 1D VO_2 rutile structure. (b) Top view of charge distribution for 1D VO_2 rutile structure. (c) Side view of charge distribution in 1D VO_2 rutile structure. (d) Side view of charge distribution in 1D VO_2 monoclinic structure.

In case of zigzag structure, VO_2(M) nanowire, exhibits two types of V-V bonds i.e. long V-V and short V-V which are present at alternate position. In VO_2 (R), each V atom makes

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bond with six O atoms and forms infinite linear chain, while in VO_2 (M) structure, each V atom makes bond with six O atoms and is stabilized to form two dimers (Figure 1). 1D VO_2(R) possesses linear V-V chains with bond length of 2.86Å, whereas zigzag structure exhibits two different types of bonds with V-V bond length 2.60Å and 3.13Å. Figure 2 shows the charge density analysis for the given VO_2 structures. The yellow surface shows the charge accumulation region for the atoms. The charge density analysis showed that the V atom form ionic bond with the O and V atom in both VO_2 NWs; however, the O atom and H atom shows covalent bond yielding sp-hybridization which prevent daggling bond in VO_2.

Electronic properties and Magnetic properties VO_2 NWs

Next, we calculate the electronic properties of the considered nanowires as shown in Figure 3. The Electronic band structure of VO_2(M) nanowire show semiconducting band gap of 1.17eV whereas, VO_2(R) nanowire is metallic in nature. Note that the band gap of bulk VO_2 is 0.7-0.9eV [44] which is in close agreements with the band gap value (1.1 eV) obtained with HSE functional [45]. The observed larger band gap in VO_2-NW is totally due to the quantum confinement effect. Note that the quatum confinement effect is observed when the diameter of a material is of the same magnitude as the de Broglie wavelength of the electron wave function. As the the size of a particle decrease, the decrease in confining dimension makes the energy levels discrete and this widen up the band gap and therefore the band gap energy also increases. The confinement effect enhanced the splitting of d-orbital in V atom of VO_2. This is why the band gap is opened up for the NW from its bulk counterpart. In VO_2(R) nanowire, the two electronic bands consists of O-2p and V-3d orbitals are found to cross Fermi level that leads to $2G_0$ ballistic conductance. Note that ballistic conductance can be obtained from the electronic band structure by counting the number of bands which crosses the Fermi level. VO_2 undergoes phase transition from monoclinic to rutile structure that leads distinctly different electronic structure. However, the reason of transition and distinct electronic properties remains in contradiction for long time [12]. The critical V-V interaction distance (R_c) for the both V^{3+}-V^{3+} and V^{4+}-V^{4+} ions is around 2.93Å [46]. The V-atoms in VO_2(M) forms dimers with two bond length value 2.60Å (which is smaller than R_c value) and 3.13Å (which is larger than R_c value). The bond length larger than R_c value leads to localization of 3d electrons. Therefore, VO_2(M) behaves as an wide gap semiconductor or insulator. On the other hand, VO_2(R) has V-V bond distance of 2.82Å, which is smaller than the R_c value. The 3d orbital electrons are shared by all metal V atoms, which are attributed to itineration of 3d electron that leads VO_2(R) to show metallic behavior. This means that the electron-electron correlations have strong influence on metal-insulator transition (MIT) process for VO_2 nanowire [47].

The PDOS for VO_2 nanowire reveals that the both valance and conduction band is contributed by V-3d and O-2p orbitals. The states around Fermi level is mainly dominated by O-2p states, while the contribution from V atom is comparatively less, which confirms the ionic bond between V-O atom and shows good agreement with our charge density analysis (Figure 2).

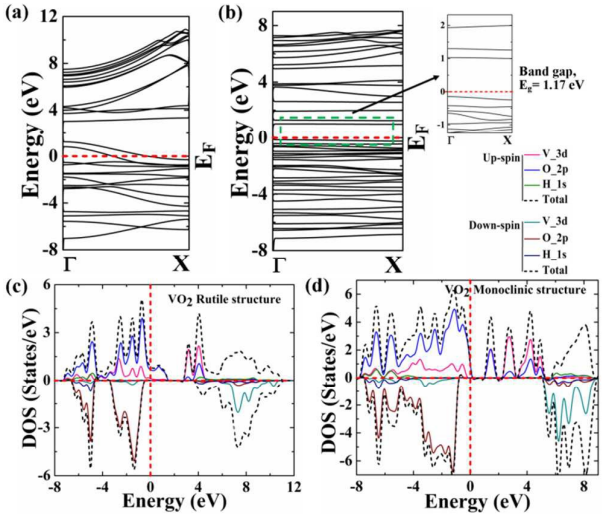

Figure 3: The calculated electronic band structure for (a) VO_2 rutile structure, (b) VO_2 monoclinic structure and corresponding partial density of states (PDOS) for (c) VO_2(R) and (d) VO_2(M). The Fermi level is at 0K.

The contribution of O-2p and V-3d at Fermi level shows p-d hybridization in both VO_2 rutile and monoclinic nanowire.

It is known that the phase transition from insulator to metal at high temperature in VO_2 induces a change in resistivity, thereby, modulate the electrical conductivity (σ) and electronic thermal conductivity (κ) of the material [16]. We have used Boltzmann transport (BoltzTrap), a semi-classical transport co-efficient approach [48], based on smoothed Fourier interpolation of band structure, to calculate the electrical and thermal conductivity.

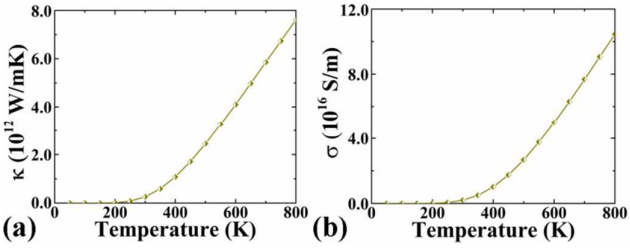

Figure 4: (a) Electronic thermal conductivity and (b) electrical conductivity of monoclinic VO_2 nanowire structure across the metal-insulator transition.

The calculated κ and σ for 1D monoclinic VO_2 as a function of temperature are shown in Figure 4. We observed that VO_2 nanowire shows zero conductivity upto 250K. Above this temperature, the thermal conductivity graph shows linear increment with temperature. The thermal conductivity increases upto $1X10^{17}$ S/m at 800K. From the κ graph, we observed the electrical conductivity for VO_2 nanowire increases with temperature above 250K and reaches to $7.6X10^{12}$ W/mK at 800K. This transition of conductivity from insulation to metallic at 250K is the transition temperature, which is much lower than the transition temperature for bulk

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VO_2. However, the phase transition from VO_2(M) to VO_2(R) can't be conformed from our calculation. The conductivity transition might be due to the collapse of electronic charge order.

Also change in the position of V atom from zigzag chain to linear chain, accompanying the evolution from the localized d-orbital electron to the delocalized state. This change in orientation of electron yields the change of spin state and magnetic moment at transition temperature. The spin polarization of VO_2 nanowire exhibits the clear picture of change in magnetic behavior. The spin polarization can be calculated from Julliere's formula [49],

$$P = \frac{D_{up-spin} - D_{down-spin}}{D_{up-spin} + D_{down-spin}} \quad (1)$$

Here P is the polarization of the material, $D_{up\text{-}spin}$ is density of states at the Fermi level due to up spin and $D_{down\text{-}spin}$ represents the density of states at Fermi level due to down spin. We observed that the spin polarization for VO_2(M) is around zero whereas, it is nearly 1 for VO_2(R) (ESI, Table S3). VO_2(M) show paramagnetic behavior whereas the metallic VO_2(R) show ferromagnetic half metal behavior. Note that it has been observed experimentally that metallic VO_2 bulk materialize into ferromagnetic structure [16]. We have also studied the magnetic moment for the VO_2 nanowire and observed that magnetic moment of 0.37μ_B for VO_2(M) changes to 0.42μ_B for VO_2(R). The change in magnetic moment corresponds to change in both magnetization and magnetic entropy. The change in magnetic properties at transition temperature is associated with the magneto-structural phase transition, which gives rise to the magnetocaloric effect (MCE). Therefore, MCE can be expected in VO_2 nanowire as it highly depends on the entropy change of the magnetic moments.

Optical properties

We now calculate the optical properties for 1D VO_2 nanowire such as refractive index, absorption and transmittance coefficient which are shown in Figure 5. In our calculations, the intraband transition due to phonon excitation is not considered, as the transition temperature is not high enough.

The refractive index curve reveals that the static refractive index, n(0), for VO_2(M) is around 0.8 and for VO_2(R), it increases to 1.4. The change in refractive index in VO_2 may be because of atomic distortion. The maximum refractive index value for monoclinic structure is calculated to be 1.27 at the photon energy of 2.37eV, which comes under visible region. Whereas, the maximum refractive index value for rutile structure is calculated to be 1.33 at 5.69eV photon energy that lies in ultra violet (UV) region. It is found that VO_2 (M) appears to have weak absorption and strong transmission in the infrared region. VO_2 (M) allows transmission of 80%-90% light in the infrared region while in the visible region (1.6-3.0eV), the transmittance curve monotonically decreases. On the other hand, the VO_2(R) turns out to have strong absorption and weak transmission in the infrared region. For E⊥chain, the absorption is observed at 0.4eV with absorption coefficient of 3×10-5cm^{-1}, whereas a flat absorption curve is observed at 2eV for E||chain (Figure 5). This change in behaviour is established due to anisotropic behaviour of VO_2. Zhang, J.et al. [18] reported the absorption curve for W adsorbed VO_2 (bulk structure) with rutile phase which is observed at 0.9eV with absorption coefficient 2×10^{-5}cm^{-1}. This yields a better absorption efficiency of VO_2 nanowire as compared to bulk structure. The transmittance curve for VO_2(R) shows monotonic decrease in the infrared region whereas a transmittance peak is observed at 2eV due to high refractive index at that region for E⊥chain.

The change in optical properties is observed as a result of existence of two different structures, monoclinic and rutile. It is to be noted that the monoclinic structure is stable at lower temperature, while the rutile structure is stable at a higher temperature. This low temperature VO_2 monoclinic structure behaves as an insulating material and allows infrared light to transmit and higher temperature VO_2 with rutile phase behaves as metallic and blocks light in the IR region. Therefore, the results show that 1D VO_2 nanowire could attract great interest as temperature sensor, optical sensor or building block for smart windows with better absorption efficiency.

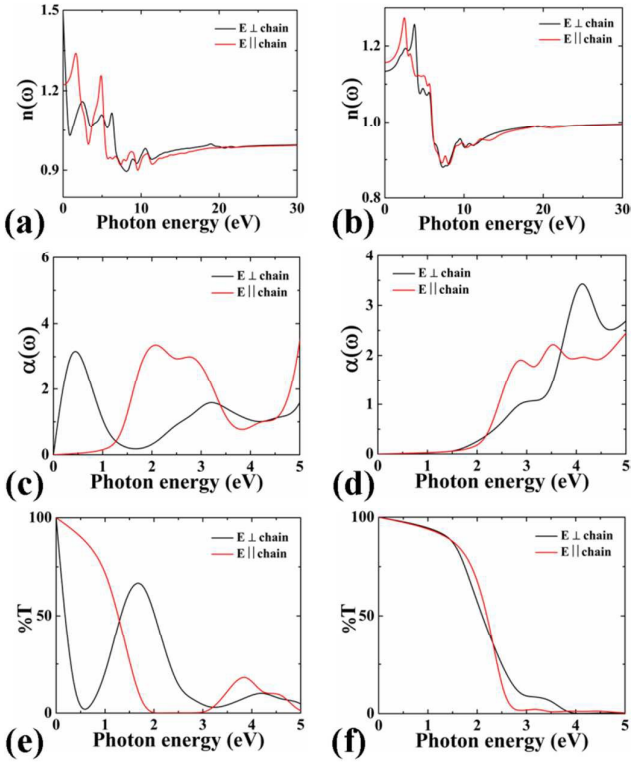

Figure 5: The calculated refractive index, absorption spectra and transmittance spectra of VO_2 rutile structure (left panel) and VO_2 monoclinic structure (right panel). The calculations are performed within random phase approximation (RPA) method along with GGA+U method.

Furthermore, we can compare the absorption spectra with the PDOS (Figure 3). Here, the valance band is dominated by O-2p

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states in both majority and minority band of VO_2(R). However the Fermi energy is dominated by V-3d and O-2p states, while the system was calculated under the consideration of spin polarization. The peaks near the Fermi energy are present at -0.67eV and -1.33eV for majority and minority band, respectively. The conduction band is mainly contributed by the V-3d states. The two major peaks are observed in majority conduction band near the Fermi level at 3.20eV due to V-3d states and at 4.05eV due to hybridized V-3d and O-2p states. The electrons in the valance band are excited to the conduction band by absorbing infrared light. The peak at 0.40eV in the absorption curve is due the transition from O-2p states in the valance band to pure V-3d states or hybridized V-3d and O-2p states in the conduction band.

Effect of molecular gas adsorption

We now consider the interaction behaviour of gaseous molecules (CO_2, N_2 and SO_2) on VO_2 (monoclinic) nanowire. We have placed the gas molecules on VO_2 nanowire at a distance of 1.5Å as shown in ESI (Figure S1). After relaxation, we found that CO_2 molecule has been stabilized at 2.06Å from the nanowire. The bond length (b) of C-O is observed to be 1.17Å. Due to interaction of CO_2 gas molecules with VO_2 nanowire, O atoms slightly tilted from C atom and make an angle of 179.16°. In case of N_2 adsorption on VO_2, the gas molecules were relaxed at distance of 2.25Å from the nanowire and the bond length was observed to be 1.09Å. The SO_2 gas molecule was stabilized at a distance of 2.04Å from the nanowire. The S-O bond length was calculated to be 1.46Å, while bond angle for SO_2 was found to be 118.30°. The adsorption energy and charge transfer due to the interaction is tabulated in Table S3. The adsorption energy (E_{ads}) of gas molecules on VO_2 nanowire is calculated from the equation;

$$E_{ads} = E_{adsorbed-NW} - (E_{VO_2-NW} + E_{adsorbent-gas}) \quad (2)$$

Where, is $E_{adsorbed\text{-}NW}$ total energy of gas molecules adsorbed on VO_2 NW $E_{VO^2\text{-}NW}$ is total energy of VO_2 NW and $E_{adsorbent\text{-}gas}$ is the total energy of respective gas molecules.

Note that, VO_2 NW considered in this study is ultrathin; the calculated adsorption energy for different positions and orientations will remain same. SO_2 gas molecule has shown high adsorption energy with -0.20eV. For N_2 and CO_2 molecules adsorbed on VO_2 NW, the adsorption energy is calculated to be -0.06eV and -0.11eV, respectively. The adsorption energy between the gas molecules and NW is directly related to charge transfer. From Lowdin charge analysis, SO_2, N_2 and CO_2 gas molecules act as charge donator which donate 0.4877e, 0.1582e and 0.2721e, respectively. The highest charge transfer in case of SO_2 gas molecules adsorbed on VO_2 NW leads to high adsorption energy. Another important feature is to study about how long the gas molecule will sustain on the nanowire. For that we have calculated relaxation time by using the equation $\tau \approx (-E_{arb}/k_BT)$; where, E_{arb} is the calculated adsorption energy, k_B is the Boltzmann constant and T is the temperature. The relaxation time for SO_2 and CO_2 gas is observed to be $2.4X10^3$ au and 1.1 $X10^2$ au, respectively. However N_2 gas shows very short relaxation time of 10.58 au, therefore it will lead to fast desorption for N_2 gas molecules from VO_2-NW surface.

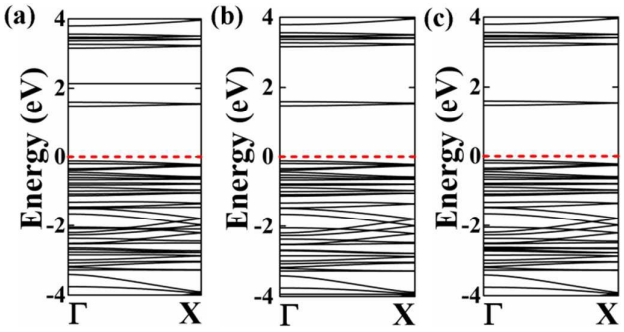

Figure 8: The electronic band structure of (a) SO_2, (b) N_2 and (c) CO_2 adsorbed VO_2(M) nanowire calculated by GGA+U method. The Fermi energy is set at 0eV.

The electronic band structure of gas molecules adsorbed on VO_2 nanowire is shown in Figure 8. We have observed that gas molecules have not influenced on the electronic band structure of VO_2(M) nanowire near the Fermi energy level that indicates the weak physiosorption of gas molecules on nanowires. The band gap has been observed to be nearly same for all three gas molecules, while in case of SO_2 molecules adsorbed on VO_2-NW, one additional band line is observed in the conduction band at 2.13eV at Γ-point.

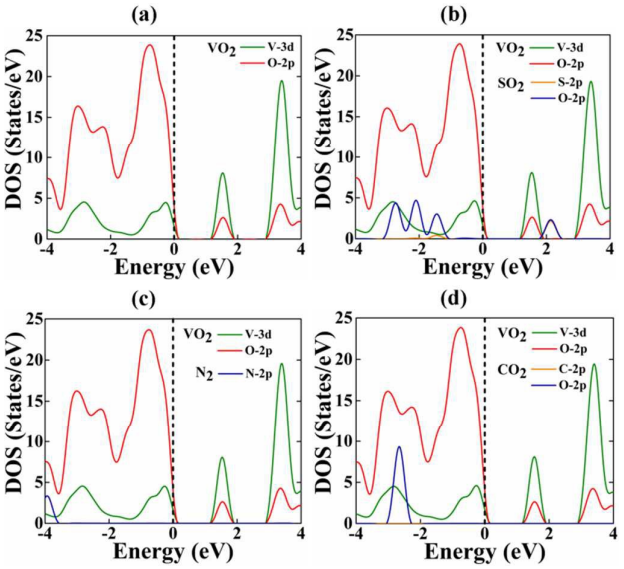

Figure 9: The partial density of states (PDOS) of (a) pure (b) SO_2, (c) N_2 and (d) CO_2 adsorbed VO_2(M) nanowire calculated by GGA+U method. The Fermi energy is set at 0eV.

For in-depth understanding of change in the electronic properties, we have turned our attention to density of states for adsorbed VO_2(M) nanowire. From PDOS graph (Figure 9), we have observed that in pure VO_2 monoclinic structure, the valance band is totally dominated by O-2p states, while the

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Fermi energy is contributed by V-3d orbitals and the conduction band is totally contributed by V-3d states. The PDOS for SO_2 adsorbed on VO_2 nanowire reveals the contribution of O-2p orbital of SO_2 in the valance band from -1.06eV to -3.12eV. An additional band that is observed in conduction band of SO_2 adsorbed VO_2 band structure, is due to the hybridized contribution of S-2p and O-2p orbital in the region from 1.78eV to 2.48eV of the same gas molecules. In case of N_2 gas molecules, the contribution of N-2p orbital is very weak. A peak of N atom is observed at -3.60eV in lower valence band, no contribution is notified in conduction band near the Fermi level region. The contribution of CO_2 molecule is observed at valence band (-2.28eV to -3.05eV). In all cases, both valance and conduction band is totally dominated by V-3d and O-2p orbital of VO_2.

The rising environmental concerns and the effect of pollution on health call for the combating this problem. The development of gas sensors for the detection of toxic gas, calculation of gas concentration in environment, breath analyzing etc. is paving a way to move forward. Here, we have discussed how VO_2 nanowire could be a good material as an optical gas sensor from the study of its absorption and transmission properties.

As we already discussed VO_2 nanowire which allows transmission of IR light in monoclinic phase at lower temperature, while at high temperature (67°C), VO_2 attains rutile structure and blocked IR light. We have introduced gas molecules like SO_2, N_2 and CO_2 on VO_2 nanowire and studied the change in optical properties of nanowire with different gas molecules. As shown in Figure 10, pure VO_2(M) nanowire shows no absorption peak in IR region. However, VO_2 nanowire in presence of SO_2 gas molecule shows absorption peak in infrared (IR) region (0.78-1.52eV) and corresponding transmission graph reveals stiff decrease in transmission compared to pure nanowire. The transmission of IR light is nearly blocked in that region. The change in the absorption peak is consequence of transfer of excited electrons from O-2p orbital of SO_2 gas to hybridized state of V-3d and O-2p orbital of VO_2 or S-2p and O-2p orbital of SO_2 gas molecules. With the introduction of N_2 gas on VO_2 nanowire, no change in absorption spectrum was observed in the IR region. This is because of weak contribution of N-2p orbital near the Fermi level region. The interaction of CO_2 gas molecules on VO_2 shows an absorption peak in the near infrared region, which leads to the change in transmission of IR light. The observed absorption peak is due to the transition from O-2p orbital of CO_2 to V-3d orbital or O-2p orbital of VO_2. The change in absorption and transmission properties in VO_2 NW due to interaction with SO_2 and CO_2 gas molecules show its strong sensitivity for sensing gas molecules, while optical properties of VO_2 nanowire is totally unaltered in the presence of N_2 gas molecules. These properties of VO_2 indicate that it has great potential application to be realized as optical gas sensors.

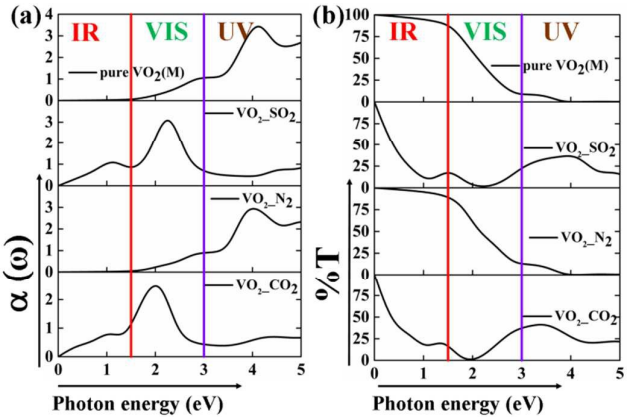

Figure 10: Comparison of absorption and transmission spectra between (a) pure VO_2 and (b) SO_2, (c) N_2 and (d) CO_2 adsorbed VO_2.

Conclusions

We have reported electronic, magnetic and optical properties for VO_2 nanowire by employing first principles calculations. The monoclinic VO_2 nanowire shows wide band gap of 1.17eV, while its rutile phase is metallic due to O-2p and V-3p orbital at Fermi level. The electronic thermal conductivity shows abrupt change in conductivity from 1.1W/mK to 8.86W/mK near transition temperature 338K. The geometric deformation of VO_2 nanowire at transition temperature leads to the change in magnetic behaviour from paramagnetic to ferromagnetic half metal. We observed that magnetic moment of 0.37 for VO_2(M) changes to 0.42 for VO_2(R). This change in magnetic moment corresponds to change in both magnetization and magnetic entropy that potentially lead to show magnetocaloric effects in nanowire. The absorption and transmission spectra of monoclinic structure of VO_2 nanowire allows infrared light to transmit, while its rutile phase blocks light in infrared region. The absorption peak is observed at 0.4eV with absorption coefficient of 3×10-5 cm^{-1} for VO_2(R) structure and this yield a better absorption efficiency of VO_2 nanowire as compared to its bulk counterpart. The VO_2(M) nanowire can be used as optical gas sensor. It offers potentially excellent sensitivity at IR region. We have shown theoretically that the gas molecules like SO_2 and CO_2 adsorbed on VO_2 nanowire can be detected from the amount of adsorption and transmission of light at IR region.

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Author contributions statements