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Highly infrared sensitive VO₂ nanowire as nano-optical device

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Recent studies on electronic, magnetic and optical properties of VO₂ (vanadium dioxide) material motivates to explore one dimensional VO₂ nanowires. First principles calculations are performed to investigate structural, electronic, magnetic and optical properties of monoclinic (M) and rutile (R) phase of VO₂ nanowire. The monoclinic phase shows semiconducting behaviour with a band gap of 1.17eV; whereas the rutile phase of VO₂ nanowire behaves as spin gapless semiconducting material, as band lines cross the Fermi level due only up spin contribution. The monoclinic structure of VO₂ nanowire is found to be paramagnetic, while the rutile structure is ferromagnetic half metal. Our conductivity calculation for VO₂ nanowire shows metal-insulator transition temperature to be 250K. The possible mechanism of VO₂ 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, VO₂ monoclinic structure allows infrared light to transmit while VO₂ with rutile phase block light in the IR region. Furthermore, we adsorbed CO₂, N₂ and SO₂ gas molecules on 1D VO₂ monoclinic nanowire to investigate their interaction behaviour. It has been observed that absorption and transmission properties of VO₂ show dramatic change on the adsorption of CO₂ and SO₂ gas molecules, which is likely to open up its application as optical gas sensor.

Introduction

Vanadium oxide (VO₂) undergoes reversible metal-insulator phase transition at 341K from monoclinic zigzag VO₂(M) structure to tetragonal rutile VO₂(R) structure [1, 2]. The geometrical deformation of VO₂ results into the change in electrical resistivity at transition temperature, thereby, shows an ability to convert thermal energy to electrical energy. Therefore, VO₂ is a promising thermoelectric material for energy harvesting [3, 4]. Furthermore, structural deformation driven transition causes change in the magnetization and optical reflectivity of VO₂, 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 VO₂ to be useful for magnetic refrigeration which is based on magneto caloric effect (MCE) [10].

In the past few decades, VO₂ 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 T_c upto 257K, while Zr-doping shows phase transition at 337.3K [13-20]. The MIT behaviour in VO₂ NW can be tuned to lower temperature by appropriate doping [21] or by axial stress [22, 23]. For example, ion diffusion in single crystalline VO₂ nanowire using ionic liquid (IL) gating has been described by change in the charge carrier concentration associated with ion doping [24]. Moreover VO₂ 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, VO₂-NW has also been studied extensively [30, 31]. Wu, X. et al. [32] reported the synthesis of VO₂ nanowire and experimentally confirmed its transition temperature to be around 341K. Furthermore, Naoi, Y. et al. [5] investigated the size of the VO₂ nanowire for transmittance efficiency. It has been reported that 1D VO₂-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 VO₂ nanowire to regulate the spin structure. VO₂ 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 VO₂ to be a potential material as transition edge sensors for gas sensing.

VO₂ material showing such interesting properties at transition temperature like MIT behaviour, abrupt change in infrared transmittance, and recent research on VO₂ 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 VO₂ 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 CO₂, N₂ and SO₂ gas molecules on VO₂(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 VO₂ 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 VO₂ nanowire, random phase approximation (RPA) method together with DFT was used. The frequency dependent complex dielectric function $\epsilon(\omega)$ can be written as $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. Here, $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ 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 VO₂, 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 VO₂ nanowire [39-43].

Results and discussions

Structural properties VO₂ NW

We have firstly relaxed tetragonal rutile, VO₂(R), and monoclinic zigzag VO₂ (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 VO₂ structure and reported V-V bond length of 2.837 Å for VO₂(R) and, 3.190 Å and 2.440 Å for VO₂(M). The both considered bulk structures are confined in y- and z-direction to have VO₂ 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, VO₂ (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.

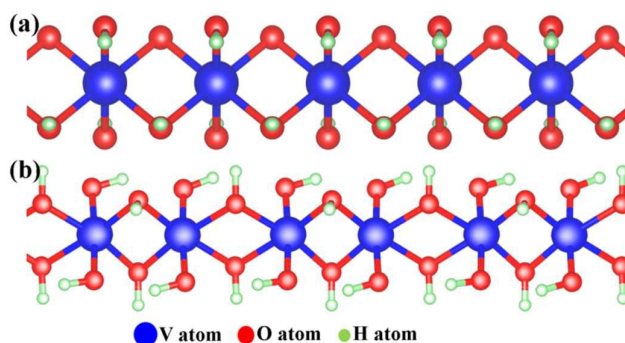


Figure 1: The optimized rutile and monoclinic structure of 1D VO₂. (a) Front view of rutile VO₂ structure. (b) Front view of monoclinic VO₂ structure.

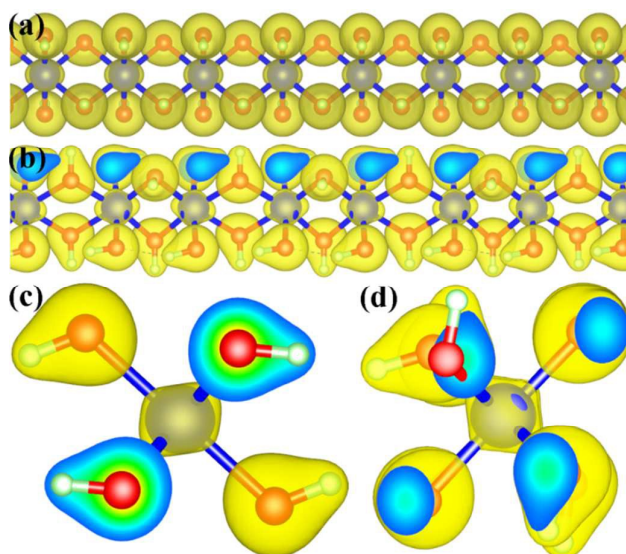


Figure 2: The calculated electronic charge density for 1D VO₂ rutile structure and 1D VO₂ monoclinic structure. (a) Top view of distribution of charge for 1D VO₂ rutile structure. (b) Top view of charge distribution for 1D VO₂ monoclinic structure. (c) Side view of charge distribution in 1D VO₂ rutile structure. (d) Side view of charge distribution in 1D VO₂ monoclinic structure.

In case of zigzag structure, VO₂(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 VO₂ (R), each V atom makes

bond with six O atoms and forms infinite linear chain, while in VO₂ (M) structure, each V atom makes bond with six O atoms and is stabilized to form two dimers (Figure 1). 1D VO₂(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 VO₂ 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 VO₂ NWs; however, the O atom and H atom shows covalent bond yielding sp-hybridization which prevent daggling bond in VO₂.

Electronic properties and Magnetic properties VO₂ NWs

Next, we calculate the electronic properties of the considered nanowires as shown in Figure 3. The Electronic band structure of VO₂(M) nanowire show semiconducting band gap of 1.17eV whereas, VO₂(R) nanowire is metallic in nature. Note that the band gap of bulk VO₂ 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 VO₂-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 VO₂. This is why the band gap is opened up for the NW from its bulk counterpart. In VO₂(R) nanowire, the two electronic bands consists of O-2p and V-3d orbitals are found to cross Fermi level that leads to 2G₀ 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. VO₂ 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 V³⁺-V³⁺ and V⁴⁺-V⁴⁺ ions is around 2.93Å [46]. The V-atoms in VO₂(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, VO₂(M) behaves as an wide gap semiconductor or insulator. On the other hand, VO₂(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 itinerant of 3d electron that leads VO₂(R) to show metallic behavior. This means that the electron-electron correlations have strong influence on metal-insulator transition (MIT) process for VO₂ nanowire [47].

The PDOS for VO₂ 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).

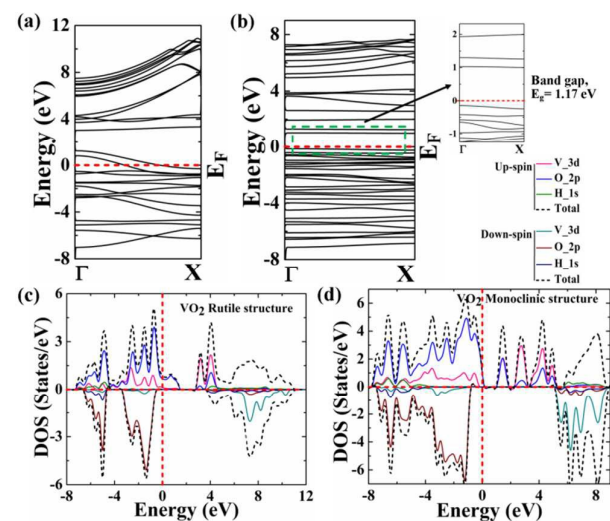


Figure 3: The calculated electronic band structure for (a) VO₂ rutile structure, (b) VO₂ monoclinic structure and corresponding partial density of states (PDOS) for (c) VO₂(R) and (d) VO₂(M). The Fermi level is at 0K.

The contribution of O-2p and V-3d at Fermi level shows p-d hybridization in both VO₂ rutile and monoclinic nanowire.

It is known that the phase transition from insulator to metal at high temperature in VO₂ 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.

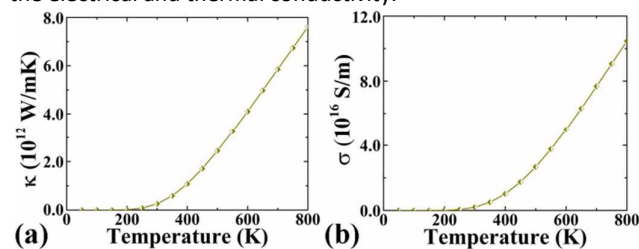


Figure 4: (a) Electronic thermal conductivity and (b) electrical conductivity of monoclinic VO₂ nanowire structure across the metal-insulator transition.

The calculated κ and σ for 1D monoclinic VO₂ as a function of temperature are shown in Figure 4. We observed that VO₂ nanowire shows zero conductivity upto 250K. Above this temperature, the thermal conductivity graph shows linear increment with temperature. The thermal conductivity increases upto 1×10^{17} S/m at 800K. From the κ graph, we observed the electrical conductivity for VO₂ nanowire increases with temperature above 250K and reaches to 7.6×10^{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

VO₂. However, the phase transition from VO₂(M) to VO₂(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 VO₂ 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, $D_{up-spin}$ is density of states at the Fermi level due to up spin and $D_{down-spin}$ represents the density of states at Fermi level due to down spin. We observed that the spin polarization for VO₂(M) is around zero whereas, it is nearly 1 for VO₂(R) (ESI, Table S3). VO₂(M) show paramagnetic behavior whereas the metallic VO₂(R) show ferromagnetic half metal behavior. Note that it has been observed experimentally that metallic VO₂ bulk materialize into ferromagnetic structure [16]. We have also studied the magnetic moment for the VO₂ nanowire and observed that magnetic moment of 0.37 μ_B for VO₂(M) changes to 0.42 μ_B for VO₂(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 VO₂ nanowire as it highly depends on the entropy change of the magnetic moments.

Optical properties

We now calculate the optical properties for 1D VO₂ 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 VO₂(M) is around 0.8 and for VO₂(R), it increases to 1.4. The change in refractive index in VO₂ 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 VO₂ (M) appears to have weak absorption and strong transmission in the infrared region. VO₂ (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 VO₂(R) turns out to have strong absorption

and weak transmission in the infrared region. For E \perp chain, the absorption is observed at 0.4eV with absorption coefficient of 3 \times 10⁻⁵cm⁻¹, whereas a flat absorption curve is observed at 2eV for E \parallel chain (Figure 5). This change in behaviour is established due to anisotropic behaviour of VO₂. Zhang, J.et al. [18] reported the absorption curve for W adsorbed VO₂ (bulk structure) with rutile phase which is observed at 0.9eV with absorption coefficient 2 \times 10⁻⁵cm⁻¹. This yields a better absorption efficiency of VO₂ nanowire as compared to bulk structure. The transmittance curve for VO₂(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 \perp 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 VO₂ monoclinic structure behaves as an insulating material and allows infrared light to transmit and higher temperature VO₂ with rutile phase behaves as metallic and blocks light in the IR region. Therefore, the results show that 1D VO₂ nanowire could attract great interest as temperature sensor, optical sensor or building block for smart windows with better absorption efficiency.

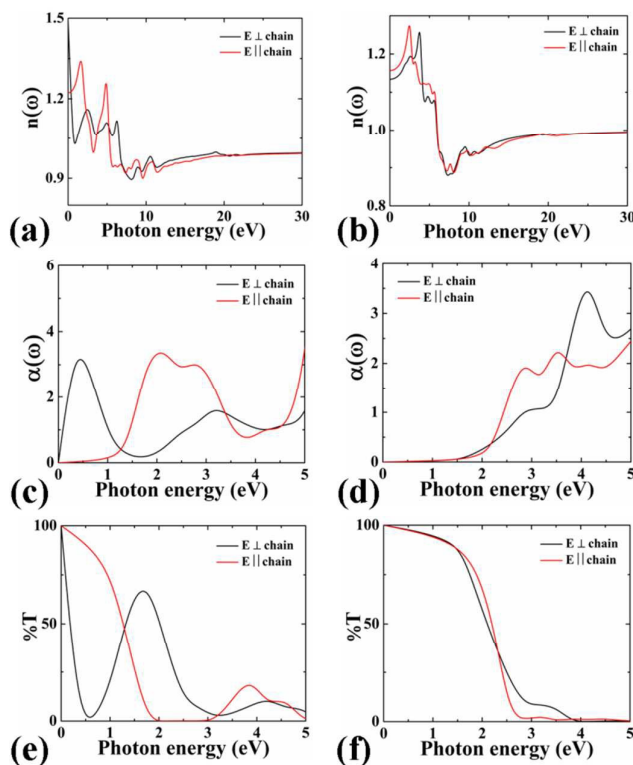


Figure 5: The calculated refractive index, absorption spectra and transmittance spectra of VO₂ rutile structure (left panel) and VO₂ monoclinic structure (right panel). The calculations are performed within random phase approximation (RPA) method along with GGA+U method.

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

states in both majority and minority band of VO₂(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 (CO₂, N₂ and SO₂) on VO₂ (monoclinic) nanowire. We have placed the gas molecules on VO₂ nanowire at a distance of 1.5Å as shown in ESI (Figure S1). After relaxation, we found that CO₂ 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 CO₂ gas molecules with VO₂ nanowire, O atoms slightly tilted from C atom and make an angle of 179.16°. In case of N₂ adsorption on VO₂, the gas molecules were relaxed at distance of 2.25Å from the nanowire and the bond length was observed to be 1.09Å. The SO₂ 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 SO₂ 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 VO₂ nanowire is calculated from the equation;

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

Where, $E_{adsorbed-NW}$ is total energy of gas molecules adsorbed on VO₂ NW, E_{VO_2-NW} is total energy of VO₂ NW and $E_{adsorbent-gas}$ is the total energy of respective gas molecules.

Note that, VO₂ NW considered in this study is ultrathin; the calculated adsorption energy for different positions and orientations will remain same. SO₂ gas molecule has shown high adsorption energy with -0.20eV. For N₂ and CO₂ molecules adsorbed on VO₂ 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, SO₂, N₂ and CO₂ gas molecules act as charge donor which donate 0.4877e, 0.1582e and 0.2721e, respectively. The highest charge transfer in case of SO₂ gas molecules adsorbed on VO₂ 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 $\tau \approx (-E_{arb}/k_B T)$; where, E_{arb} is the calculated adsorption energy, k_B is the Boltzmann constant and T is the temperature. The relaxation time for SO₂

and CO₂ gas is observed to be 2.4×10^3 au and 1.1×10^2 au, respectively. However N₂ gas shows very short relaxation time of 10.58 au, therefore it will lead to fast desorption for N₂ gas molecules from VO₂-NW surface.

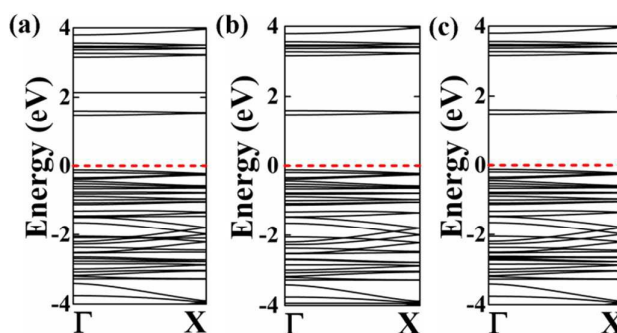


Figure 8: The electronic band structure of (a) SO₂, (b) N₂ and (c) CO₂ adsorbed VO₂(M) nanowire calculated by GGA+U method. The Fermi energy is set at 0eV.

The electronic band structure of gas molecules adsorbed on VO₂ nanowire is shown in Figure 8. We have observed that gas molecules have not influenced on the electronic band structure of VO₂(M) nanowire near the Fermi energy level that indicates the weak physisorption of gas molecules on nanowires. The band gap has been observed to be nearly same for all three gas molecules, while in case of SO₂ molecules adsorbed on VO₂-NW, one additional band line is observed in the conduction band at 2.13eV at Γ -point.

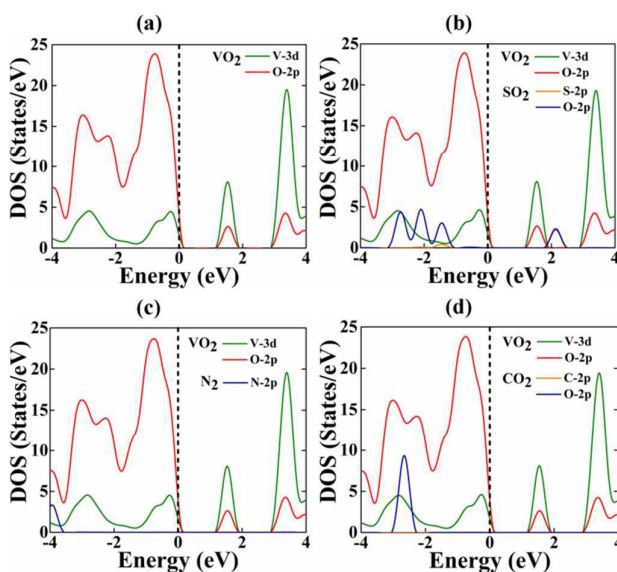


Figure 9: The partial density of states (PDOS) of (a) pure (b) SO₂, (c) N₂ and (d) CO₂ adsorbed VO₂(M) nanowire calculated by GGA+U method. The Fermi energy is set at 0eV.

For in-depth understanding of change in the electronic properties, we have turned our attention to density of states for adsorbed VO₂(M) nanowire. From PDOS graph (Figure 9), we have observed that in pure VO₂ 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 SO₂ adsorbed on VO₂ nanowire reveals the contribution of O-2p orbital of SO₂ in the valance band from -1.06eV to -3.12eV. An additional band that is observed in conduction band of SO₂ adsorbed VO₂ 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 N₂ gas molecules, the contribution of N-2p orbital is very weak. A peak of N atom is observed at -3.60eV in lower valance band, no contribution is notified in conduction band near the Fermi level region. The contribution of CO₂ molecule is observed at valance 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 VO₂.

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 VO₂ nanowire could be a good material as an optical gas sensor from the study of its absorption and transmission properties.

As we already discussed VO₂ nanowire which allows transmission of IR light in monoclinic phase at lower temperature, while at high temperature (67°C), VO₂ attains rutile structure and blocked IR light. We have introduced gas molecules like SO₂, N₂ and CO₂ on VO₂ nanowire and studied the change in optical properties of nanowire with different gas molecules. As shown in Figure 10, pure VO₂(M) nanowire shows no absorption peak in IR region. However, VO₂ nanowire in presence of SO₂ 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 SO₂ gas to hybridized state of V-3d and O-2p orbital of VO₂ or S-2p and O-2p orbital of SO₂ gas molecules. With the introduction of N₂ gas on VO₂ 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 CO₂ gas molecules on VO₂ 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 CO₂ to V-3d orbital or O-2p orbital of VO₂. The change in absorption and transmission properties in VO₂ NW due to interaction with SO₂ and CO₂ gas molecules show its strong sensitivity for sensing gas molecules, while optical properties of VO₂ nanowire is totally unaltered in the presence of N₂ gas molecules. These properties of VO₂ indicate that it has great potential application to be realized as optical gas sensors.

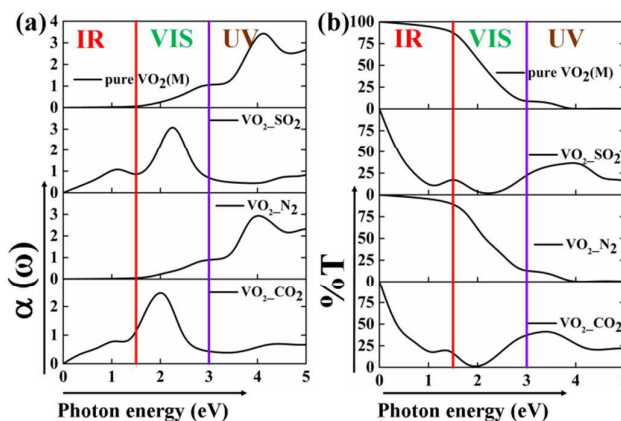


Figure 10: Comparison of absorption and transmission spectra between (a) pure VO₂ and (b) SO₂, (c) N₂ and (d) CO₂ adsorbed VO₂.

Conclusions

We have reported electronic, magnetic and optical properties for VO₂ nanowire by employing first principles calculations. The monoclinic VO₂ 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 VO₂ 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 VO₂(M) changes to 0.42 for VO₂(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 VO₂ 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 VO₂(R) structure and this yield a better absorption efficiency of VO₂ nanowire as compared to its bulk counterpart. The VO₂(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 SO₂ and CO₂ adsorbed on VO₂ nanowire can be detected from the amount of adsorption and transmission of light at IR region.

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Author contributions statements

"PDB and SKG were associated with the DFT calculations and prepared Figures and wrote the main manuscript text. AK, YAG and PNG helped to improve the scientific content of the article. All authors reviewed the manuscript."

Competing financial interests

The author(s) declare no competing financial interests.

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