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Novel $Zn_2(V,Nb,Ta)N_3$ Monolayers for Application in Tandem Solar Cells

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INTRODUCTION & AIM

The discovery of novel nanomaterials with outstanding functionality remains paramount for continuous technological advancements. Recently, significant attention has been paid to a family of zinc-based ternary nitrides. For instance, a comprehensive computational study demonstrated of hundreds of new (meta)stable ternary nitrides.[1]

Zhuk et al. synthesized the Zn_2VN_3 thin film following computational simulations.[2] The Zn_2VN_3 thin film has a wide band gap of 2.35 eV, high charge carrier concentration of $\sim 10^{17}$ cm^{-3}, and Hall mobility of 80 $cm^2/(V \cdot s)$, which make it a promising candidate for application in solar cells.

In this work, using first-principles simulations mechanical and optical properties and chemical activity towards nitrogen gas molecules of novel ternary nitride $Zn_2(V,Nb,Ta)N_3$ monolayers are studied.

METHOD

The calculations were performed in the frame work of density functional theory (DFT). The Perdew−Burke−Ernzerhof (PBE) functional[3] under the generalized gradient approximation (GGA) was used for the geometry optimization and mechanical properties calculations. Optical properties were calculated using the hybrid exchange-correlation functional HSE06[4]. The plane-wave basis cutoff energy was set to 540 eV. Periodic boundary conditions were implemented in the in-plane transverse directions, while a vacuum space of 20 Å was introduced to the out-of-plane direction. The van der Waals interaction upon NO and NO_2 gas molecules adsorption was treated using the DFT-D3 dispersion correction.

RESULTS & DISCUSSION

The predicted $Zn_2(V,Nb,Ta)N_3$ monolayers reflect light in the far-infrared and infrared regions from 0.1 to 1.65 eV and absorb light in the visible range. The maximum absorption value reaches 16.06%, 17.46% and 17.72% for the Zn_2VN_3, Zn_2NbN_3, and Zn_2TaN_3 monolayers (Figures 1a-c), respectively. Moreover, the Zn_2VN monolayer possesses the highest strength and elasticity (Figures 1d-f).

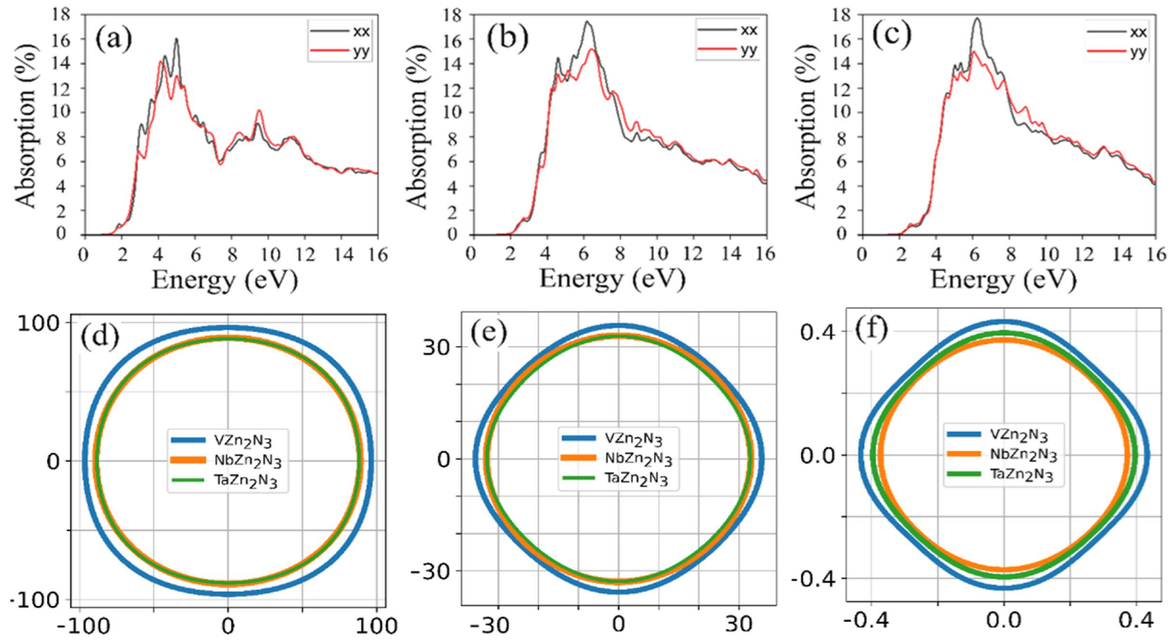

Figure 1. Absorption spectra A(ω) of the (a) Zn_2VN_3, (b) Zn_2NbN_3, and (c) Zn_2TaN_3 monolayers in xx (black line) and yy (red line) directions. Spatial dependencies of (d) Young's modulus (N/m), (e) shear modulus (N/m), and (f) Poisson's ratio for the $Zn_2(V,Nb,Ta)N_3$ monolayers.

In addition, the Zn_2VN_3 monolayer is the most stable in moisty environment and is less reactive towards atmospheric N-containing gas molecules It is also found that there is a the local surface dipole (Figure 2a,b) at the interface between the $Zn_2(V,Nb,Ta)N_3$ monolayers and the NO and NO_2 molecules, which affects their functionality.

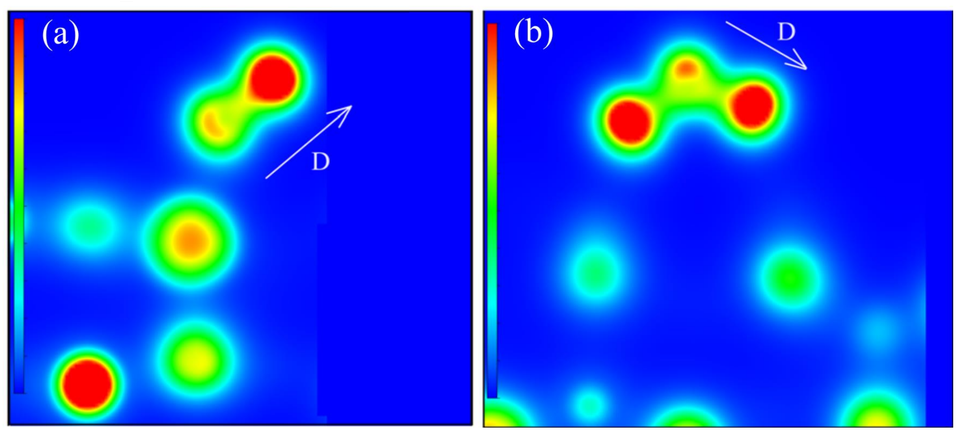

Figure 2. Electron localization function for (a) NO and (b) NO_2 on the $Zn_2(V,Nb,Ta)N_3$ monolayers. D denotes dipole moment.

CONCLUSION

The Zn_2VN_3 monolayer is the most promising for application in solar energy devices, for instance, as blocking layers in tandem solar cells. The Zn_2TaN_3 monolayers is found to be promising for application in molecular sensing.

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