Supporting Information

First principles calculation of the ZnV_2O_6(001) surface terminations: the thermodynamics stability and electronic structure study

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1. Calculation Details

The surface Gibbs free energy is a function of different atomic chemical potentials and represents the excess energy of a semi-infinite crystal in contact with the reservoir material compared to the bulk crystal. Calculating the surface Gibbs free energy allows one to examine the stability of the surface under environmental conditions while taking the exchange of atoms between the crystal, the surface, and the gas into account[1]. For constant pressure and constant temperature, the most stable surface termination minimizes the surface Gibbs free energy. ZnV_2O_6's surface Gibbs free energy is written as $\Omega(ZnV_2O_6)$ as in [1-4].

$$\Omega(ZnV_2O_6) = \frac{1}{2}\left(G_{ZnV_2O_6}^{slab} - n_{Zn}\mu_{Zn} - n_V\mu_V - n_O\mu_O\right) \quad (1)$$

Here, Gslab ZnV_2O_6 is the Gibbs free energy of the surface. μ_i(i = Zn, V, O) is the chemical potential of the atoms Zn, V and O that make up ZnV_2O_6. n_{Zn}, n_V and n_O are the number of Zn, V and O atoms. The coefficient 1/2 indicates that there are two surface sides for each surface termination.

As the slab oxides on the upper and lower surfaces are in thermal equilibrium, the chemical potential (μ_{Zn}, μ_V and μ_O) According to equation (3), the Gibbs free energy of bulk ZnV_2O_6 is thermodynamically correlated with each other [1-4].

$$\mu_{ZnV_2O_6} = \mu_{Zn} + 2\mu_V + 6\mu_O = g_{ZnV_2O_6}^{bulk} \quad (2)$$

The chemical potential of ZnV_2O_6 is equal to the bulk crystal Gibbs free energy since the surface of each plate is in equilibrium with the ZnV_2O_6 crystal (in its standard states). This results in the expression

$$g_{ZnV_2O_6}^{bulk} = E_{ZnV_2O_6}^{bulk} \quad (3)$$

According to Eqs. (4)-(6), the individual chemical potentials can be represented in terms of the isolated atomic energy E_i and the relative change in chemical potential $\Delta\mu_X$(X=Zn, V, O). The chemical potential's variance does, however, fall within a certain range of viability.

For example, $\Delta\mu_O$ is the chemical potential subject to oxygen-poor conditions (indicating the onset of ZnV_2O_6 bulk formation after the presence of vanadium and zinc bulk in the oxygen-phase reservoir.

Conversely, it also shows that ZnV_2O_6 bulk has a propensity to break down into its component metals/metal oxides and oxygen, and that this process is limited by oxygen (indicating the condensation of O_2 gas on the surface). Here, the oxygen-poor limit is arbitrarily taken into account as the enthalpy of metal oxide formation[5, 6]. Depending on the corresponding bulk and the surrounding macroscopic composition of the individual bulk oxides, Zn or V can either be enriched or depleted.

$$\Delta\mu_{Zn} = \mu_{Zn} - E_{Zn}^{bulk} \tag{4}$$

$$\Delta\mu_{V} = \mu_{V} - E_{V}^{bulk} \tag{5}$$

$$\Delta\mu_{O} = \mu_{O} - \frac{1}{2}E_{O_2} \tag{6}$$

Here, E_{Zn}^{bulk}, E_{V}^{bulk} and E_{O_2} are the total energy per atom of bulk Zn, V and O_2 molecules calculated by DFT.

It must be noted that in Equation 1, the $\Omega(ZnV_2O_6)$ dependence is imposed by μ_{Zn}, μ_V and μ_O. We take $\Delta\mu_V$ and $\Delta\mu_O$ as independent variables. When μ_{Zn} is replaced by μ_V and μ_O through Equation (1). can be written as Equation (7).

$$\Omega(ZnV_2O_6) = \phi - \frac{1}{2}(n_V - 2n_{Zn})\Delta\mu_V - \frac{1}{2}(n_O - 6n_{Zn})\Delta\mu_O \tag{7}$$

where

$$\phi = \frac{1}{2}(G_{ZnV_2O_6}^{slab} - n_{Zn}E_{ZnV_2O_6}^{bulk}) - \frac{1}{2}(n_V - 2n_{Zn})E_{V}^{bulk} - \frac{1}{2}(n_O - 6n_{Zn})\frac{E_{O_2}}{2} \tag{8}$$

$E_{ZnV_2O_6}^{slab}$ is the total energy of ZnV_2O_6 bulk. The number of O and Bi atoms related to Zn atoms in the surface model is the coefficient of $\frac{1}{2}(n_V - 2n_{Zn})$ and $\frac{1}{2}(n_O - 6n_{Zn})$, which indicate the degree of excess of the number of Zn atoms for the surface termination compared to the slab model, respectively.

A border that prevents metal Zn, V from precipitating on the surface is necessary to identify the stability zone of ZnV_2O_6. Additionally, oxygen atoms should not be allowed to combine to produce oxygen molecules. Consequently, the line separating the chemical potentials of Zn and V is

$$\Delta\mu_{Zn} \leq 0 \tag{9}$$

$$\Delta\mu_{V} \leq 0 \tag{10}$$

The oxygen atom's chemical potential, which differs from its energy in the free, isolated O_2 molecule

$$\Delta\mu_{O} \leq 0 \tag{11}$$

The upper bound of the chemical potentials of Zn, V, and O is defined by the inequality (9–10). The lower boundary can be determined by combining equation (2) and inequalities (9–10) to arrive at the following formula.

$$2\Delta\mu_v + 6\Delta\mu_o \geq \Delta g_f(ZnV_2O_6)$$
(12)

Zn and V oxide deposition must be prevented by additional boundary requirements.

$$\Delta\mu_{Zn} + \Delta\mu_V \leq \Delta g_f(ZnO) \quad (13)$$

$$2\Delta\mu_{Zn} + 5\Delta\mu_V \leq \Delta g_f(V_2O_5) \quad (14)$$

$$\Delta\mu_v + 2\Delta\mu_o \leq \Delta g_f(VO_2) \quad (15)$$

$\Delta g_f(ZnV_2O_6)$ has the meaning of the Gibbs free energy of formation for ZnV_2O_6 from Zn, V, and O2 in their standard states. The Gibbs free energies of bulk formation are $\Delta g_f(ZnO)$, $\Delta g_f(V_2O_5)$, and $\Delta g_f(VO_2)$.The total energy of bulk V_2O_5, ZnO, and VO_2 is designated as $E^{bulk}_{V_2O_5}$, E^{bulk}_{ZnO}, and $E^{bulk}_{VO_2}$, respectively. once more by merging the equation's boundary conditions:

$$\Delta g_f(V_2O_5) \geq 2\Delta\mu_V + 5\Delta\mu_O \geq \Delta g_f(ZnV_2O_6) - \Delta g_f(ZnO) \quad (16)$$

$$\Delta g_f(ZnO) = E^{bulk}_{ZnO} - E^{bulk}_{Zn} - \frac{1}{2}E_{O_2} \quad (17)$$

$$\Delta g_f(V_2O_5) = E^{bulk}_{V_2O_5} - 2E^{bulk}_{V} - \frac{5}{2}E_{O_2} \quad (18)$$

$$\Delta g_f(VO_2) = E^{bulk}_{VO_2} - E^{bulk}_{V} - E_{O_2} \quad (19)$$

Where $\Delta g_f(ZnV_2O_6)$ is the Gibbs free energy of formation of ZnV_2O_6

$$\Delta g_f(ZnV_2O_6) = E^{bulk}_{ZnV_2O_6} - E^{bulk}_{Zn} - 2E^{bulk}_{V} - 3E_{O_2} \quad (20)$$

At the crystal surface, the oxygen atoms in ZnV_2O_6 are assumed to be in equilibrium with the oxygen in the surrounding air, resulting in equivalent oxidation potentials for both the crystal and the environment.

$$\mu_O = \frac{1}{2}\mu_{O_2} \quad (21)$$

It is difficult to obtain the oxidation potential under experimental and industrial conditions. Oxygen can be thought of as an ideal gas because its chemical potential is dependent on the temperature and pressure of the gas. The chemical potential of oxygen can be stated as[2, 7] using the ideal gas theory.

$$\mu_{O_2}(T,P) = \mu_{O_2}(T,P^0) + kTln(\frac{P}{P^0}) \quad (22)$$

where p^0 is the reference pressure used as the standard pressure and k is the Boltzmann constant, $8.617x10^{-5}$ eV/K(1atm). We use the reference condition of an isolated oxygen molecule E_{O2} and can express the divergence of the oxidation potential as

$$\Delta\mu_O(T,P) = \mu_O(T,P) - \frac{1}{2}E_{O_2} \quad (23)$$

We note the deviation of oxidizing chemical components to avoid time-consuming and difficult calculations.

$$\Delta\mu_O(T,P) = \frac{1}{2}[\Delta G_{O_2}^{gas} + kTln(\frac{P}{P^0})] + \delta\mu_O^0 \quad (24)$$

Here, Δg(T, p) is the change in oxygen's Gibbs free energy with respect to temperature at standard pressure p^0 and temperature T^0=298.15K, which can be found in the NIST-JANAF thermodynamics table[8]. Table 3 displays the derived values of Δg(T, p). The adjustment term $\delta\mu_O^0$ can be expressed as follows in order to make the calculation and experimental results consistent:

$$\delta\mu_O^0 = \frac{1}{y}(E_{M_xO_y}^{bulk} - xE_M^0 - \frac{1}{N_A}\Delta H_{f,M_xO_y}^0) - \frac{1}{2}T^0S_{O_2}^0 - \frac{1}{2}E_{O_2}^{gas} \quad (25)$$

Where, M_xO_y and M represent V_2O_5, VO_2 or ZnO oxide and Zn or V metal, respectively. Their formation enthalpies $\Delta H_{f,M_xO_y}^0$ and standard oxygen entropy $T^0S_{O_2}^0$ were obtained from thermodynamic data[4]. In order to match the DFT calculation and experimental change of O_2, the correction $\delta\mu_O^0$ is introduced into the equation. Our findings show that an average value of 0.03 eV is employed.

Table S1 Variation in Gibbs free energy for oxygen gas at standard pressure with respect to its value at 0 K. Information was derived from the NIST-JANAF table[8].

T (K)	$GgasO_2$ (T, p^0)(eV)
100	-0.150
200	-0.341
298	-0.544
300	-0.548
350	-0.655
400	-0.765
450	-0.877
500	-0.991
600	-1.222
700	-1.460
800	-1.702
900	-1.949
1000	-2.199
1100	-2.453
1200	-2.711
1300	-2.972
1400	-3.235
1500	-3.501

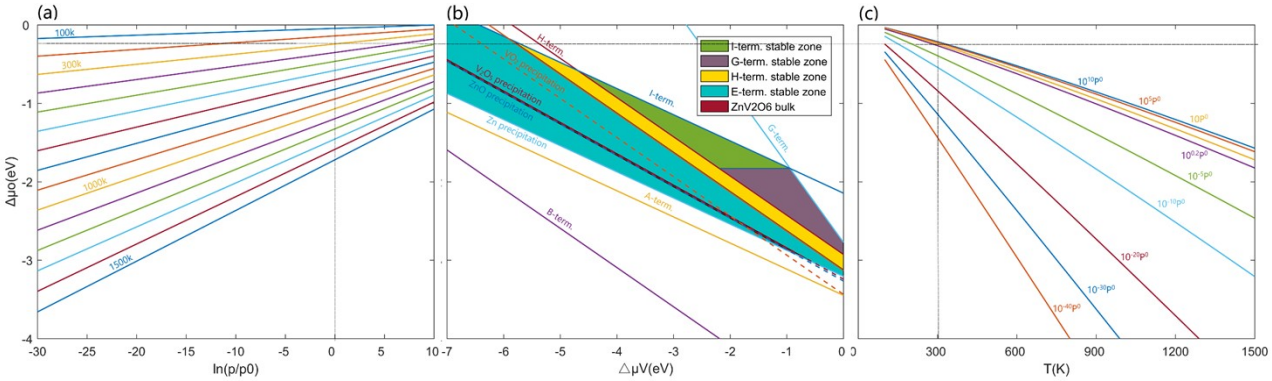

Figure S1 $\Delta\mu_O$ as a function of oxygen pressure at different temperatures (a), phase diagrams at different terminations (A, B, C, D, E, F, G, H, I) surfaces as a function of vanadium and oxygen atomic chemical potential changes (b), $\Delta\mu_O$ as a function of temperature at different oxygen pressures (c)

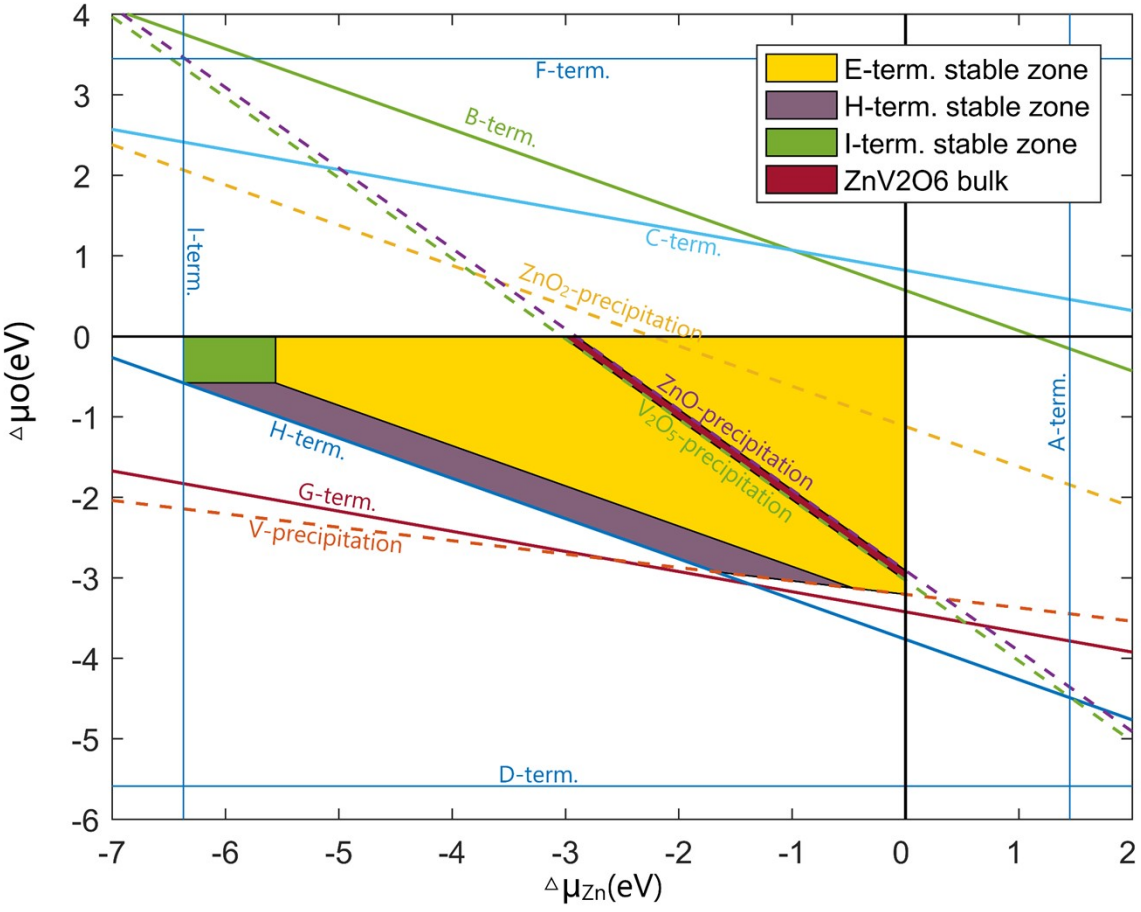

Figure S2 the phase diagrams at different terminations (A, B, C, D, E, F, G, H, I) surfaces as a function of zinc and oxygen atomic chemical potential changes

2. Atomic displacement after optimization

Table S2 Atom Displacement of the Topmost Layers of Nine Terminated Surfaces (Only the top 10 layers are shown)

E		G		H		I	
bond	drel (%)	bond	drel (%)	bond	drel (%)	bond	drel (%)
O3-V	-0.91%	V-O3	-1.03%	O2-V	0.40%	O1-V	0.96%

V-O2	0.49%	V-O3'	4.20%	V-O3	1.19%	O2-V	-0.20%
V-O1	0.29%	V-O2	-3.12%	V-O3'	0.67%	V-O3	0.02%
O1-Zn	2.14%	V-O1	-0.07%	V-O2	-1.50%	V-O3'	-0.43%
Zn-O1	1.60%	Zn-O1	-1.37%	V-O1	0.49%	V-O2	-0.25%
Zn-O2	0.16%	Zn-O2	0.61%	Zn-O1	1.10%	V-O1	0.28%
O1-V	0.37%	V-O3	-0.38%	Zn-O2	0.91%	Zn-O1	-3.28%
O2-V	-0.15%	V-O3'	0.72%	V-O3	0.95%	Zn-O2	0.26%
V-O2	-0.37%	V-O3	-0.09%	V-O3'	0.80%	V-O3	-0.59%
V-O1	0.05%	V-O3'	0.43%	V-O2	-0.23%	V-O3'	0.39%

$$d_{rel} = \frac{\Delta Z^{origin}_{i,j} - \Delta Z^{relaxed}_{i,j}}{\Delta Z_0}$$

$\Delta Z^{origin}_{i,j}$ is the distance between atoms i and j in the non-relaxed plate, $\Delta Z^{relaxed}_{i,j}$ relaxation is the distance between atoms i and j in the relaxed plate, and ΔZ_0 is the unit cell length of the ZnV_2O_6 crystal. For d_{rel}, the plus sign means shrinkage between the surface layers, while the minus sign means expansion.

The CONTCAR of E:

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V O Zn

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  0.5225210127655942  0.2795004608702314  0.3667075047924797
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The CONTCAR of G:

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The CONTCAR of H:

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V O Zn

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