Support Information

For

Role of oxygen impurity on the mechanical stability and atomic cohesion of Ta_3N_5 semiconductor photocatalyst

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The elastic constants of orthorhombic crystals are calculated using the method proposed by Ravindran[1], et al. Since the calculation procedures of all elastic constants are almost identical, we then only use c_{44} as an example to conduct a detailed discussion.

If we apply following distortion matrices

$$\begin{pmatrix} \frac{1}{(1-\delta^2)^{1/3}} & 0 & 0 \\ 0 & \frac{1}{(1-\delta^2)^{1/3}} & \frac{\delta}{(1-\delta^2)^{1/3}} \\ 0 & \frac{\delta}{(1-\delta^2)^{1/3}} & \frac{1}{(1-\delta^2)^{1/3}} \end{pmatrix} \quad \text{(S-1)}$$

to the lattice of Ta_3N_5 (where δ is lattice strain), the total energy of Ta_3N_5 associated with this distortion can be expressed as:

$$E(V,\delta) = E(V_0,0) + V_0(2\tau_4\delta + 2c_{44}\delta^2) \quad \text{(S-2)}$$

where V_0 and $E(V_0,0)$ are the volume and total energy of the unstrained Ta_3N_5, respectively, and τ_4 is the strain tensor. It is seen that, the elastic constants c_{44} can be extracted from the second derivative of the total energy $E(V,\delta)$. With the lattice strain δ varying from -0.01 to 0.01 (interval = 0.0025), we can get corresponding total energies $E(V,\delta)$. The dependence of total energy $E(V,\delta)$ on the lattice strain δ is shown in Fig. S1. Based on the second-order polynomial fit, the value of $2V_0c_{44}$ is determined. After dividing $2V_0c_{44}$ by $2V_0$, we can get the elastic constant c_{44}.

After obtaining all elastic constants, the bulk modulus (B), shear modulus (G) and Young's modulus (E) can be derived from the Voigt-Reuss-Hill approximation[2]. More calculation details of modulus please refer to Ravindran[1], et al.'s work. Using above mentioned energy-strain method, elastic constants and bulk modulus of Ta_2N_3 are calculated and listed in Table S1. It is seen that, except the c_{66}, all our calculated elastic constants are in good agreement with other theoretical results[3]. The discrepancy in c_{66} between our results and other theoretical work may be ascribed to: (i) our calculation method is the energy-strain method, while the method in Ref. 3 is the stress-strain method; (ii) the stress amplitude used in our calculation varies from -0.01 to 0.01, which may be different from that in Ref. 3. However, the discrepancy in c_{66} does not affect the bulk modulus calculation, because bulk modulus calculation does not need c_{66}. Our calculated B of Ta_2N_3 is 327 GPa, which is in good agreement with the result in Ref. 3 and the experimental value (319 GPa)[4].

References

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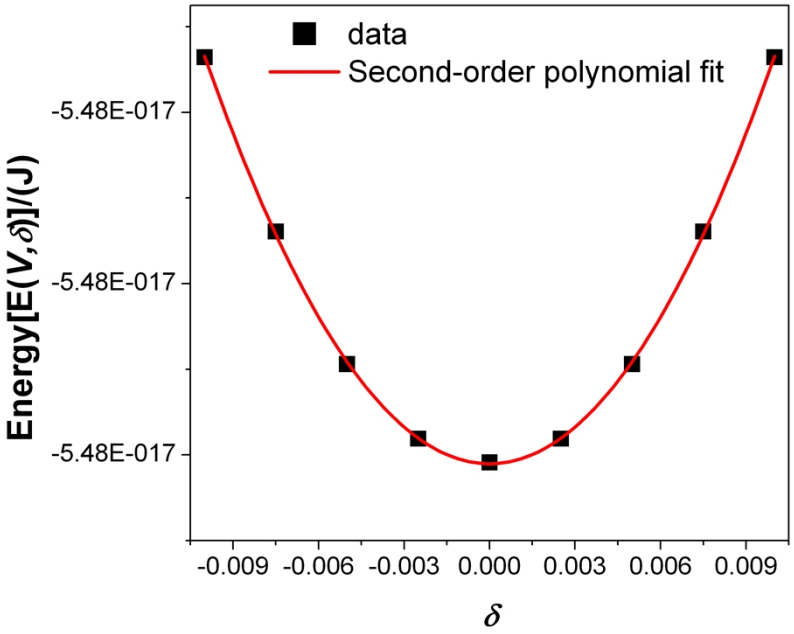

Fig. S1. Dependence of total energy $E(V,\delta)$ on the lattice strain δ.

Table S1. Calculated single-crystal elastic constants c_{ij} (GPa) and polycrystalline bulk modulus B (GPa) of Ta_2N_3.

	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}	B^a
This work	465	611	640	166	192	-115	245	199	177	327
Ref. 3	456	610	639	165	193	-54	245	203	176	327

[a] Exp[4]. = 319 GPa