

Supplementary Material

High-Electron-Affinity Oxides V_2O_5 Enhances Surface Transfer Doping on Hydrogen-Terminated Diamond

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1. V₂O₅ doped VdP diamond devices

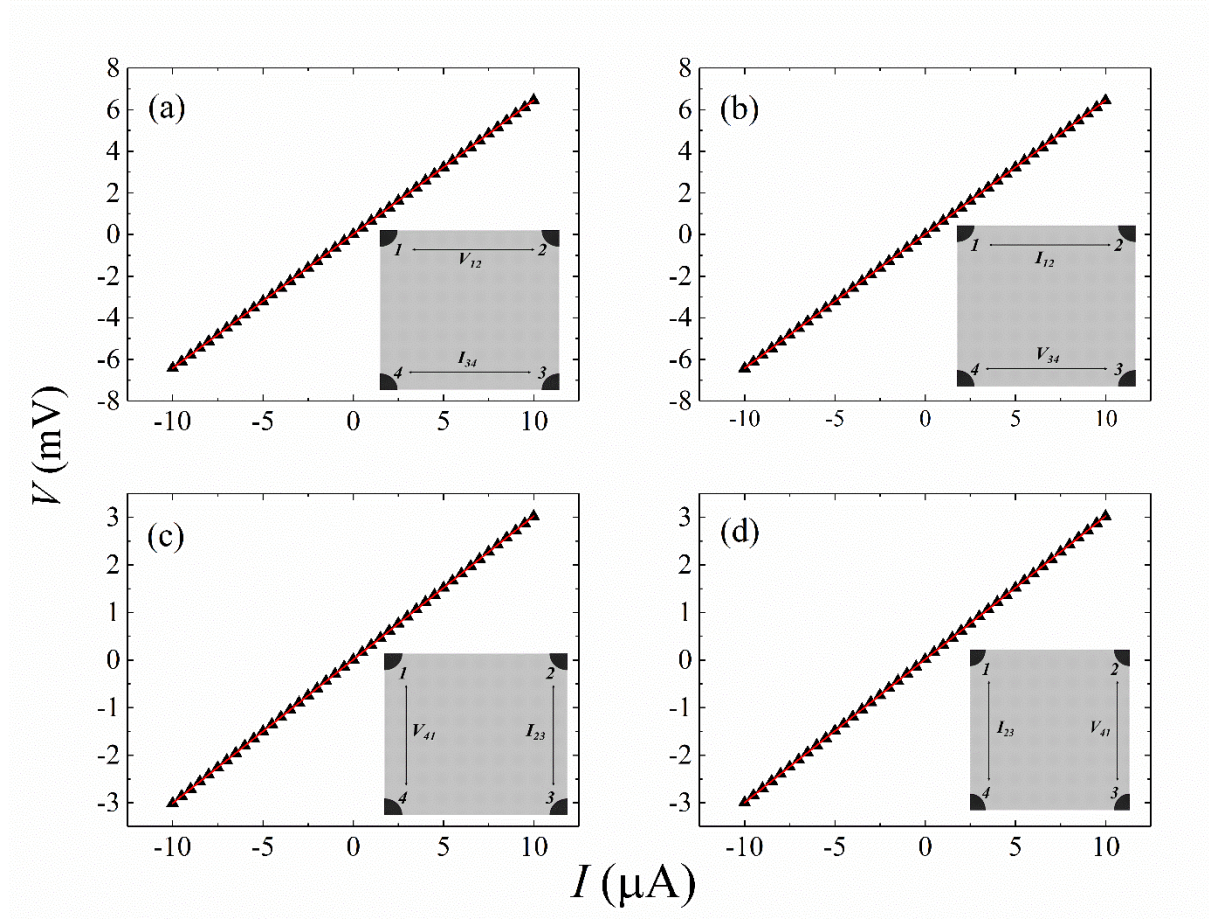


Figure S1. I - V curves for sheet resistance measurements of V₂O₅ doped hydrogen-terminated diamond in VdP configuration.

The sheet resistance can be calculated by:

$$\exp\left(-\frac{\pi \cdot R_A}{R_{\text{sheet resistance}}}\right) + \exp\left(-\frac{\pi \cdot R_B}{R_{\text{sheet resistance}}}\right) = 1 \quad \text{Eq. (S0)}$$

The values of R_A and R_B can be determined as follow:

$$R_A = \left(\frac{V_{34}}{I_{12}} + \frac{V_{12}}{I_{34}} \right) / 2$$

$$R_B = \left(\frac{V_{41}}{I_{23}} + \frac{V_{24}}{I_{41}} \right) / 2$$

2 Empirical relationship between ρ_{xx} and n_{2D}

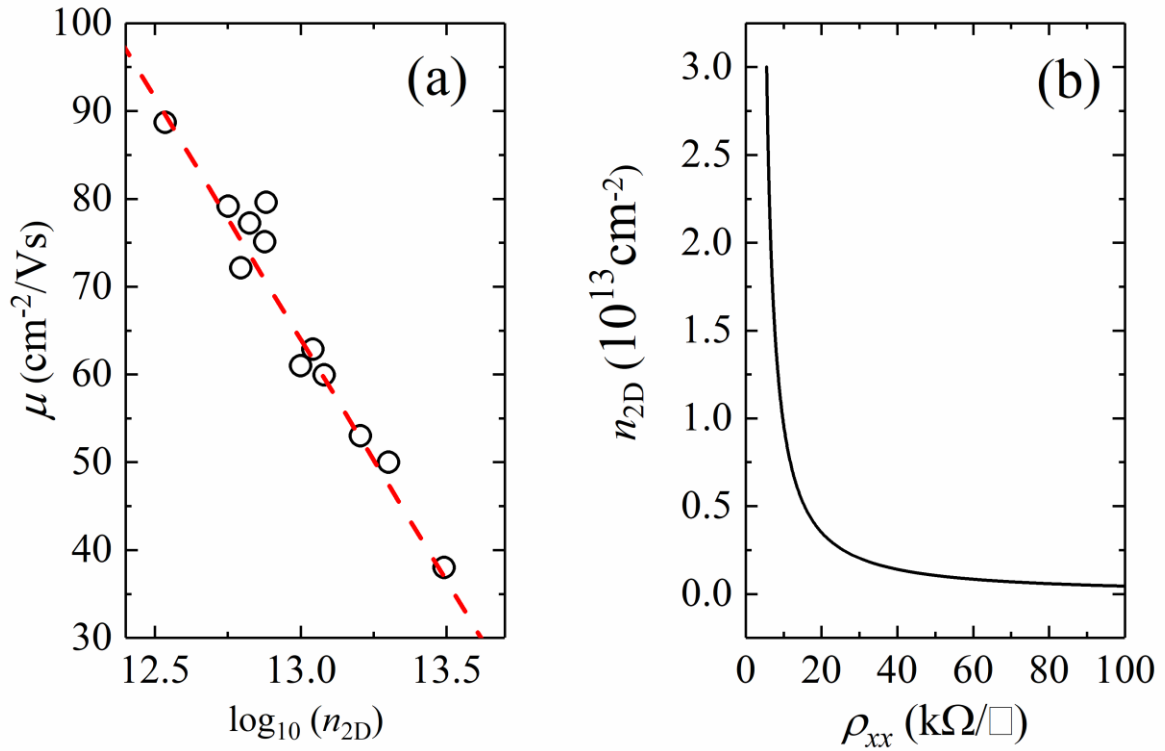


Figure S2. (a) Carrier mobility plotted as a function of carrier density, showing logarithmic carrier density dependence. (b) Empirical relationship between hole carrier density and sheet resistance.

3. Areal hole density as a function of the surface valence band position u_s

The hole density at the diamond surface depends on the position of E_V^{Diamond} relative to Fermi energy at the diamond surface, $u_s = E_V^{\text{Diamond}} - E_F$. It can be derived from Poisson's equation as follows [1]:

$$n_{2D}(u_s) = \sqrt{\frac{2kT\epsilon_r\epsilon_0 N_V}{e^2}} \cdot e^{\frac{u_s}{2kT}} \quad \text{Eq. (S1)}$$

For the non-degenerate case $u_s < 0$ and

$$n_{2D}(u_s) = \sqrt{\frac{2kT\epsilon_r\epsilon_0 N_V}{e^2}} \cdot \sqrt{1 + \frac{u_s}{kT} + \frac{8}{15\sqrt{\pi}} \left(\frac{u_s}{kT}\right)^{\frac{5}{2}}} \quad \text{Eq. (S2)}$$

For the degenerate case when $u_s > 0$. n_{2D} represents the hole density. N_v is the effective density of states in the valence band of diamond, and it is equal to $3 \times 10^{19} \text{ cm}^{-3}$ at room temperature. ϵ_0 and ϵ_r represents the vacuum permittivity and the dielectric constant of diamond, which is $8.854 \times 10^{-12} \text{ F/m}$ and 5.8, respectively. k and T are the Boltzman constant and temperature.

4. Optimized structures for the considered configurations of hydrogen-terminated diamond surface with V_2O_5 adsorption

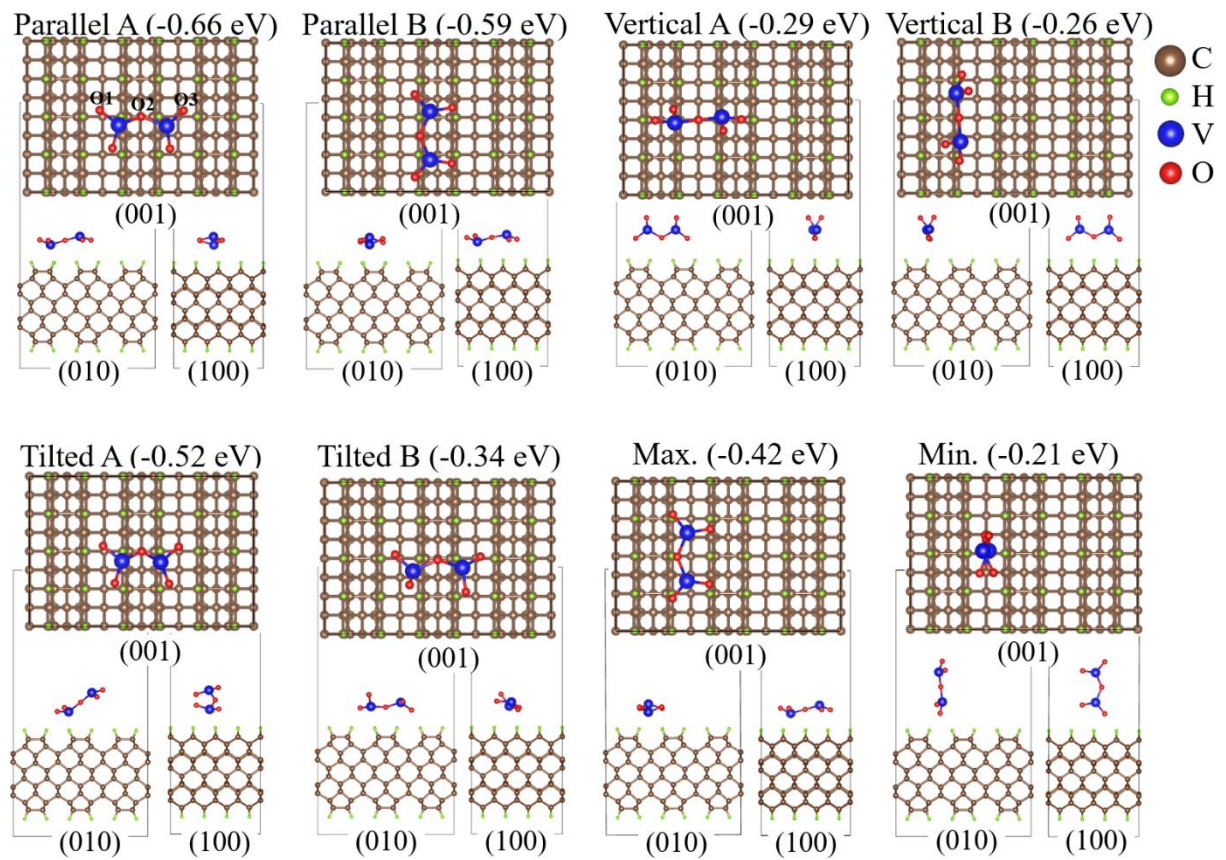


Figure. S3 Schematic view of the optimized structures for the considered configurations of hydrogen-terminated diamond surface with V_2O_5 adsorption

The corresponding adsorption energies are listed in the parenthesis. For parallel, tilted and vertical doping, the normal direction of the three-oxygen (O1, O2 and O3) surface is parallel, tilted and perpendicular to the diamond surface, respectively. For the four parallel and vertical-typical cases, we consider 6 structures (the central O atom in different position including 1st, 2nd, 3rd and 4th layer C, top of H and bridge of two 1st layer C) and only show the most stable

structure for every type of cases. Based on the results of parallel cases we consider the two tilted cases with different inclination angles and show the most stable structure. The cases of maximum (Max.) and minimum (Min.) to form the O-H bond are also considered. The blue, red, brown and green spheres represent V, O, C and H atoms, respectively.

Reference

- [1] Ley, L. Surface Conductivity of Diamond. *In CVD Diamond for Electronic Devices and Sensors*, Ricardo S. Sussmann; John Wiley & Sons Ltd. United Kingdom, 2009, 69–102.