

Supplementary material

MoO₃ induces *p*-type Surface Conductivity by Surface Transfer Doping in Diamond

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1. 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]:

$$n_{2D}(u_s) = \sqrt{\frac{2kT\epsilon_r\epsilon_0N_V}{e^2}} \cdot e^{\frac{u_s}{2kT}} \quad \text{Eq. (S1)}$$

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

$$n_{2D}(u_s) = \sqrt{\frac{2kT\epsilon_r\epsilon_0N_V}{e^2}} \cdot \sqrt{1 + \frac{u_s}{kT} + \frac{8}{15\sqrt{\pi}} \left(\frac{u_s}{kT}\right)^{\frac{5}{2}}} \quad \text{Eq. (S2)}$$

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.

2 Schematic views of the configurations of MoO₃-doped hydrogen-terminated diamond surface

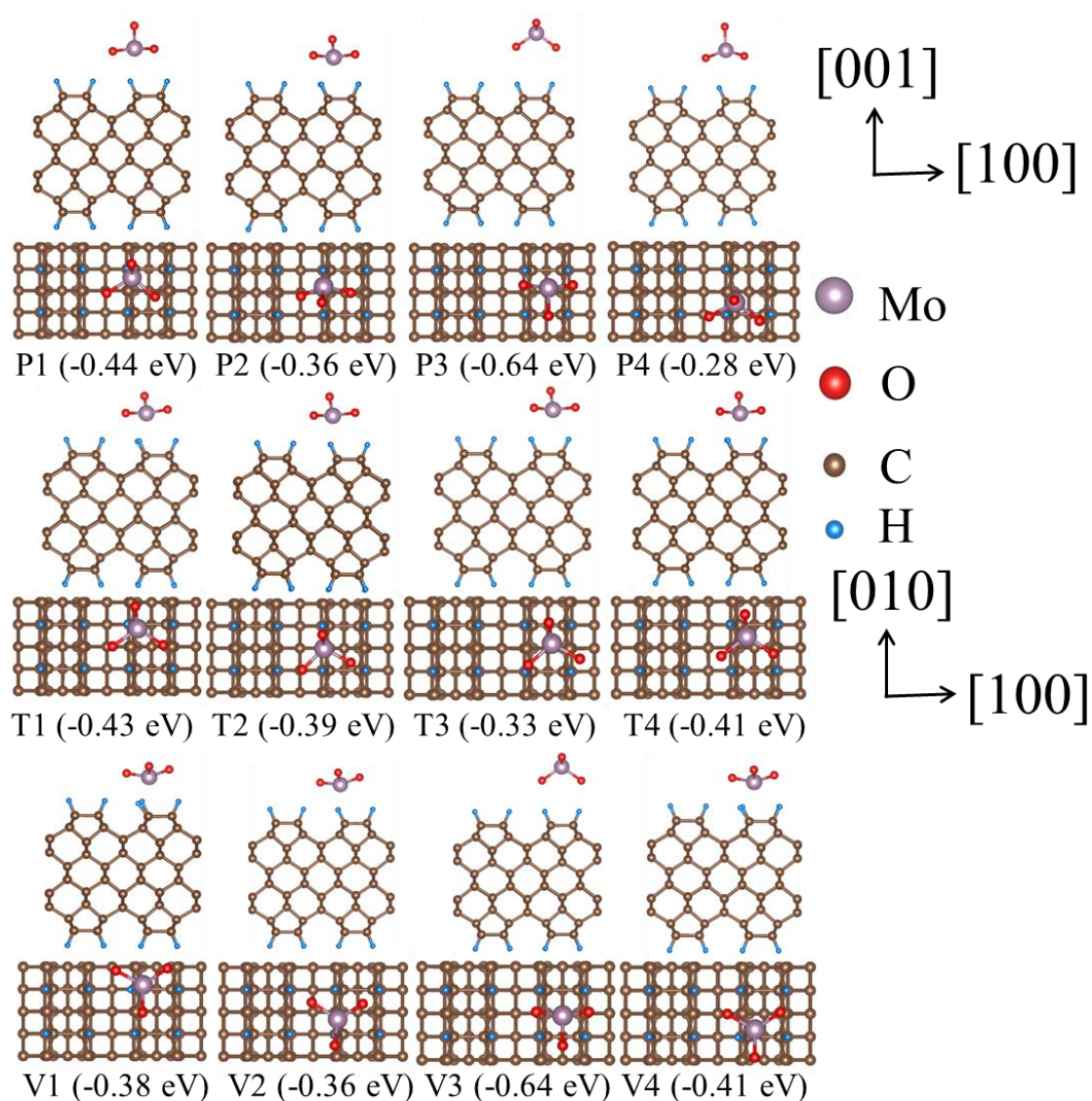


Figure S1. Schematic view of the optimized structures for the considered configurations of hydrogen-terminated diamond surface with MoO_3 adsorption. The corresponding adsorption energies are listed in the parenthesis. For parallel (P), tilted (T) and vertical (V) doping, the normal direction of the three-oxygen plane is parallel, tilted and perpendicular to the diamond surface, respectively. The gray, red, brown and light blue spheres represent Mo, O, C and H atoms, respectively.

3. Empirical relationship between hole density and sheet resistance

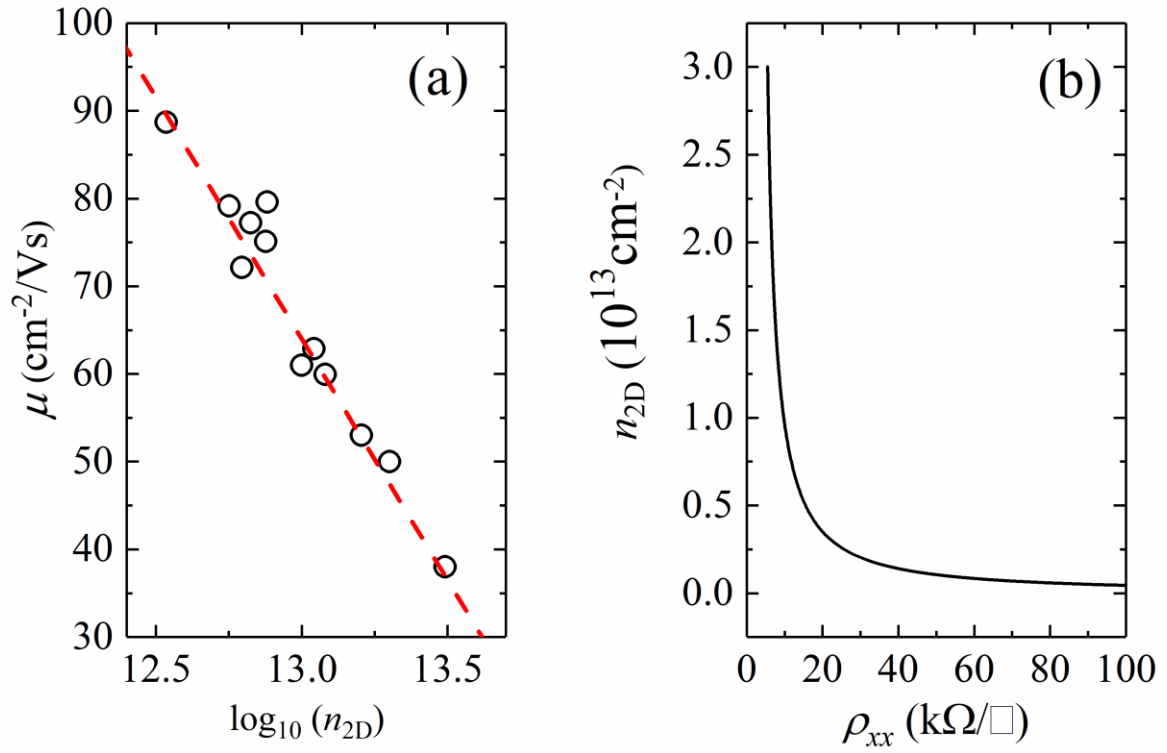


Figure S2. (a) Carrier mobility plotted as a function of carrier density, showing logarithmic carrier density dependence. (b) Empirical relationship between hole carrier density and sheet resistance.

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.