Steric Gating Directs Room-Temperature Hydrosilylation on Silicon Hydride Surfaces

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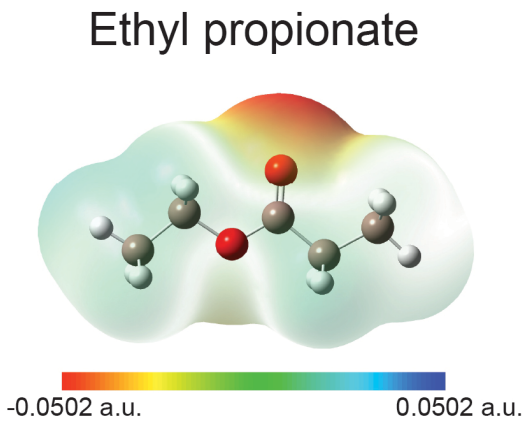
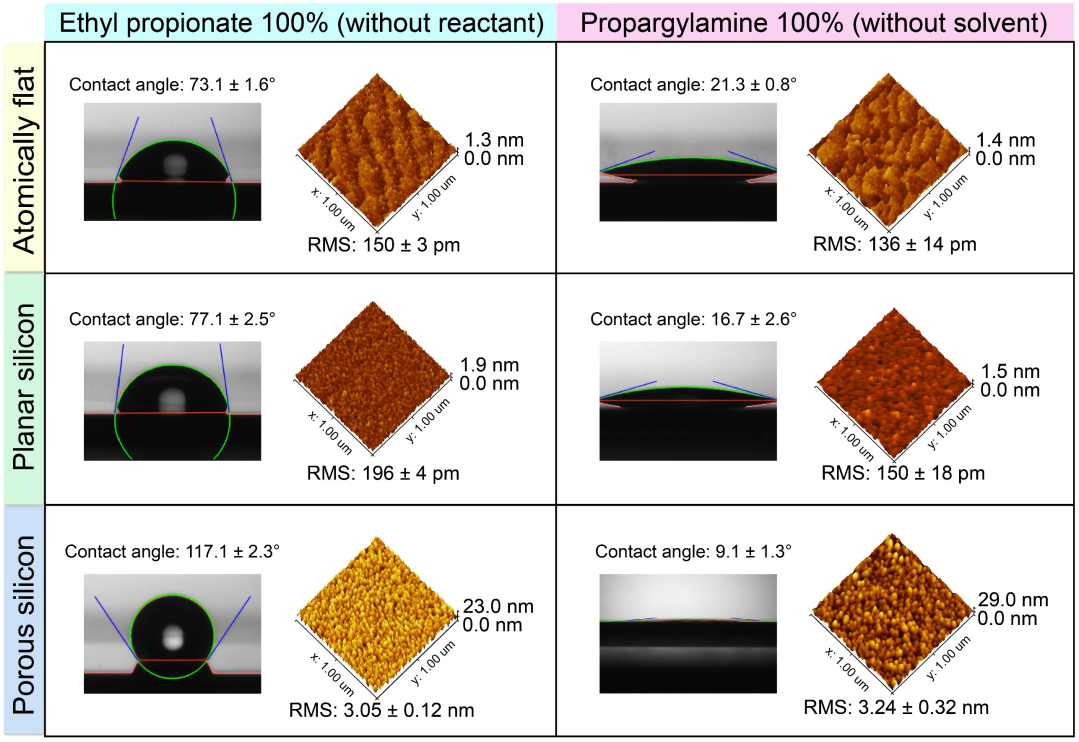
Supplementary information

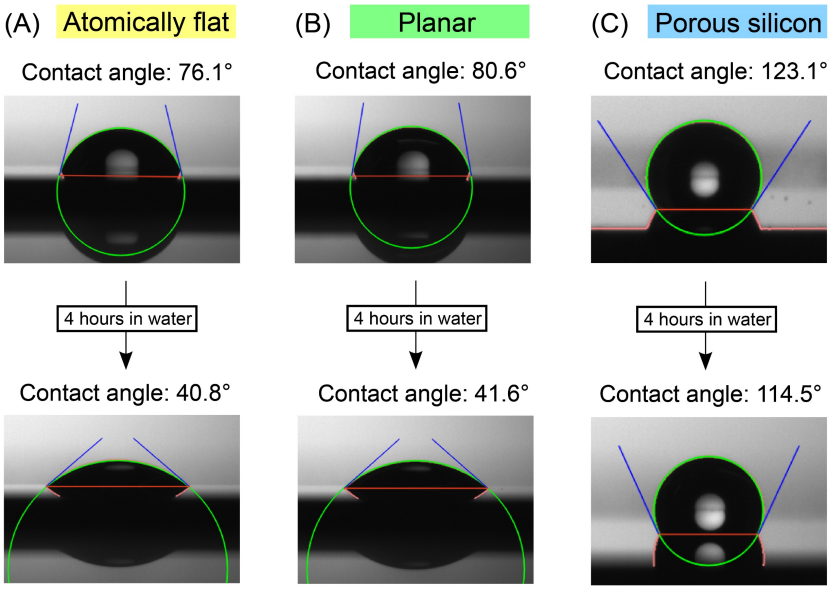


Calculation Method	RB3LYP	
Basis Set	6-311++G(D,P)	
Charge	0	
Spin	Singlet	
Solvation	None	
Electronic Energy	-347.13	Hartree
Dipole Moment	1.93	Debye

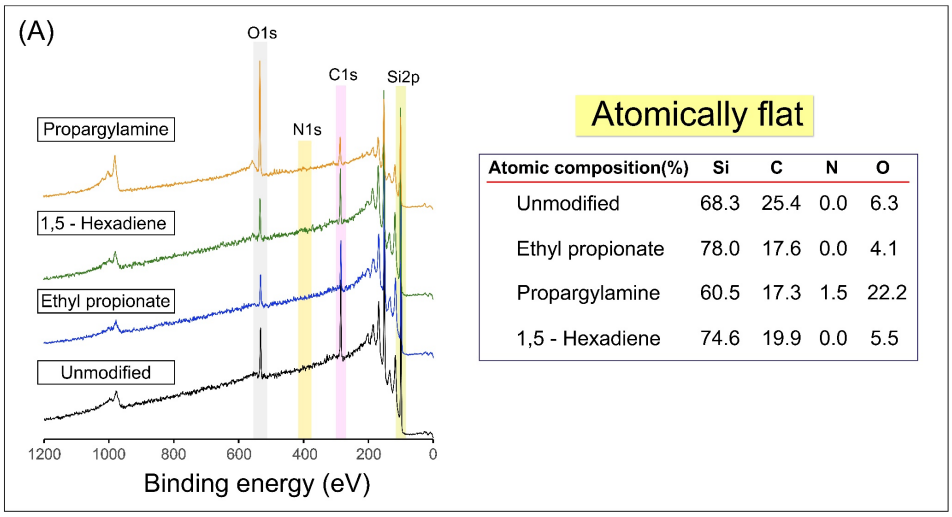
Supplementary Figure 1. ESP surface and dipole moment of ethyl propionate calculated at the RB3LYP/6-311++G(d,p) level. The electrostatic potential is mapped onto the electron density isosurface (0.005 a.u.), with colors representing potential values as shown in the scale bar.



Supplementary Figure 2. This study investigates the neat reactions of ethyl propionate and propargylamine to evaluate the roughening effect on three types of silicon surfaces. Notably, the porous silicon surface exhibits a pronounced roughening effect during the propargylamine neat reaction.

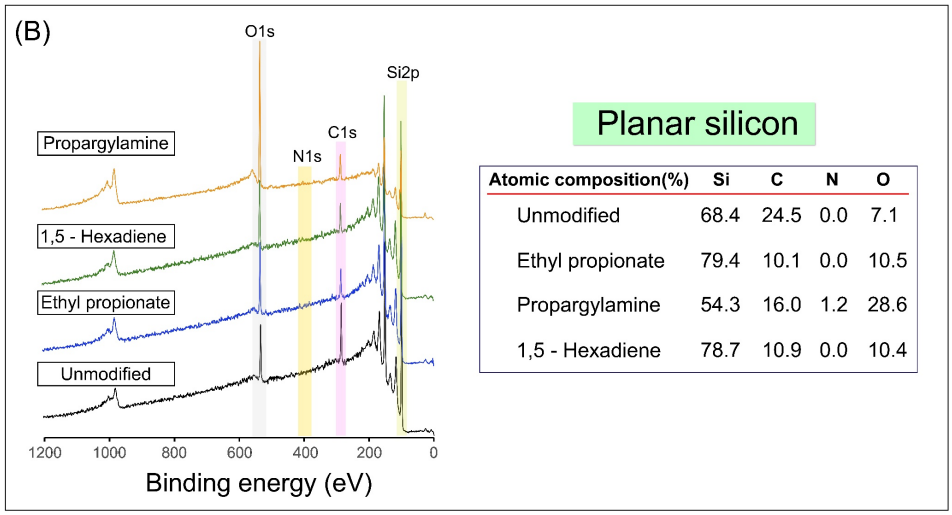


Supplementary Figure 3. Contact angle measurements conducted before and after 4-hour immersion in water indicate no significant variation in surface wettability, with all samples demonstrating comparable behavior to the propargylamine-modified surface.



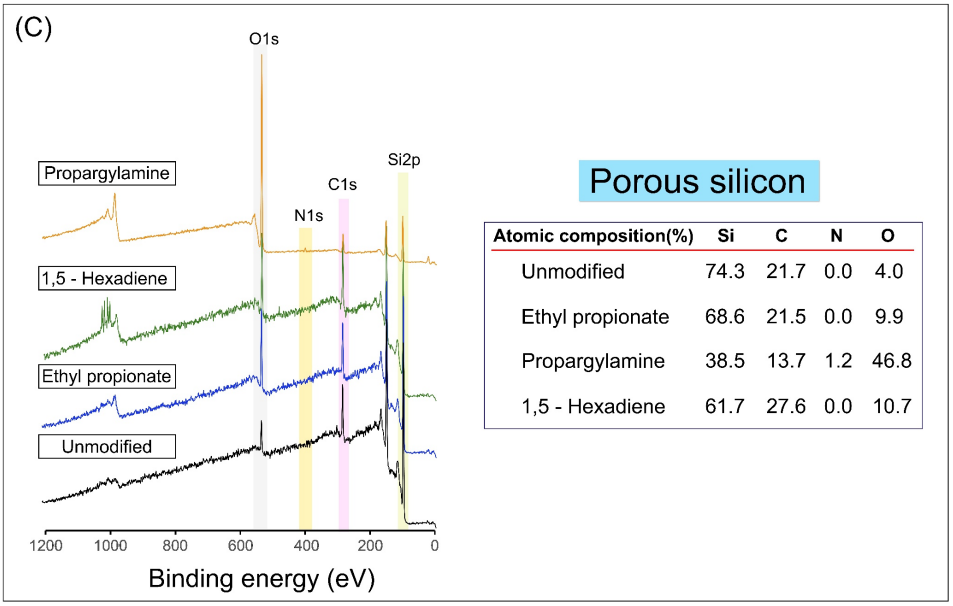
Atomically flat

Atomic composition(%)	Si	C	N	O
Unmodified	68.3	25.4	0.0	6.3
Ethyl propionate	78.0	17.6	0.0	4.1
Propargylamine	60.5	17.3	1.5	22.2
1,5 - Hexadiene	74.6	19.9	0.0	5.5



Planar silicon

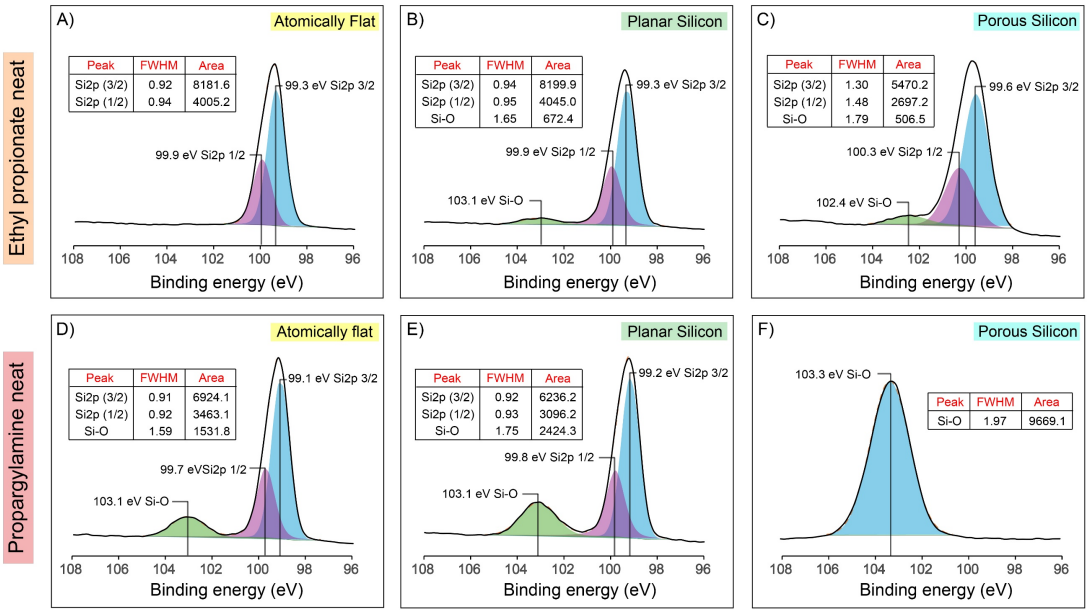
Atomic composition(%)	Si	C	N	O
Unmodified	68.4	24.5	0.0	7.1
Ethyl propionate	79.4	10.1	0.0	10.5
Propargylamine	54.3	16.0	1.2	28.6
1,5 - Hexadiene	78.7	10.9	0.0	10.4



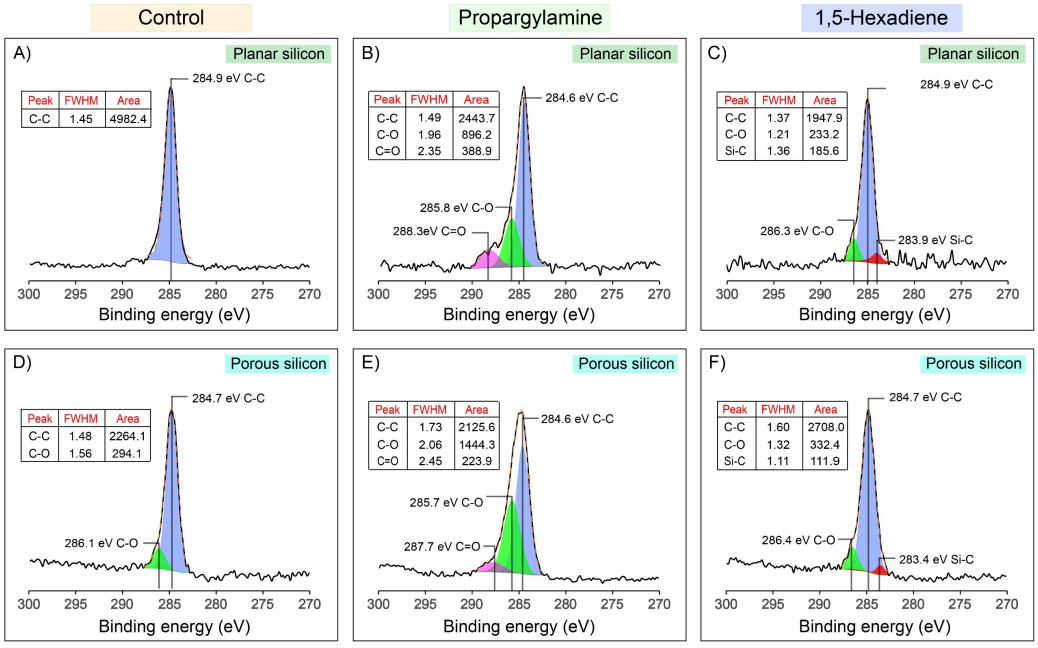
Porous silicon

Atomic composition(%)	Si	C	N	O
Unmodified	74.3	21.7	0.0	4.0
Ethyl propionate	68.6	21.5	0.0	9.9
Propargylamine	38.5	13.7	1.2	46.8
1,5 - Hexadiene	61.7	27.6	0.0	10.7

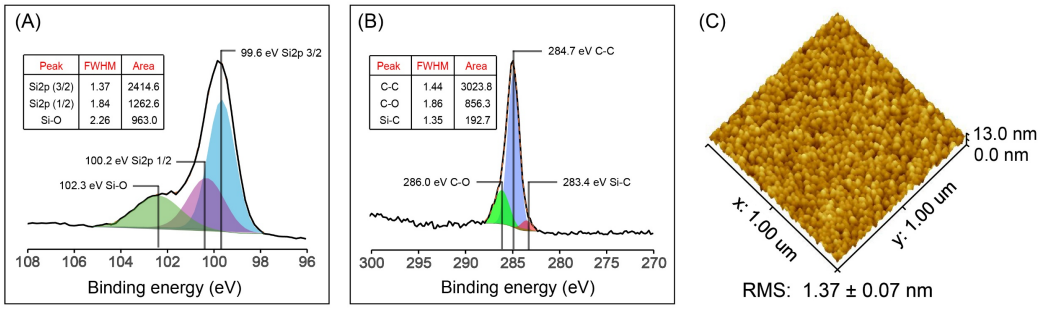
Supplementary Figure 4. X-ray photoelectron spectroscopy (XPS) survey spectra of (A) atomically flat, (B) planar, and (C) porous silicon surfaces, before and after surface modification.Each panel displays the unmodified surface and surfaces treated with ethyl propionate alone or in combination with propargylamine or 1,5-hexadiene. Key elemental peaks (Si, C, N, O) are highlighted.



Supplementary Figure 5. High-resolution XPS Si2p spectra of silicon surfaces after reaction with neat ethyl propionate (top row: A–C) and neat propargylamine (bottom row: D–F). Peak positions, full width at half maximum (FWHM), and integrated areas are listed in the insects, highlighting variations in surface oxidation and bonding environments across different morphologies and reagents.



Supplementary Figure 6. High-resolution XPS C1s spectra of planar and porous silicon surfaces after different surface treatments: Spectra were deconvoluted into individual components representing C–C, C–O, and Si–C bonding environments.



Supplementary Figure 7. High-resolution XPS Si2p and C1s spectra of porous silicon after modified with propiolic. Atomic force microscopy (AFM) topography image (1 × 1 μm²), displaying a rough surface morphology with an RMS roughness of 1.37 ± 0.07 nm.