

Supporting Information

Theoretical Prediction of Silicether: A Two-Dimensional Hyperconjugated Disilicon Monoxide Nanosheet

Gui-Lin Zhu^{||}, Xiao-Juan Ye^{||}, Chun-Sheng Liu^{*}, and Xiao-Hong Yan

College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China

^{||}The first two authors contributed equally to this work.

^{*}E-mail: cslu@njupt.edu.cn

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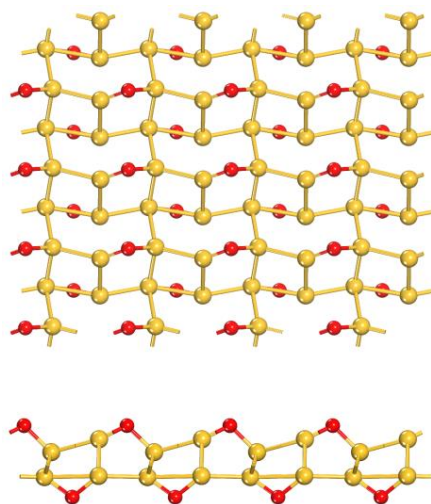


Figure S1. Snapshots for the final configurations of silicether after ~ 0.3 ps AIMD simulations with temperature at 1000 K.

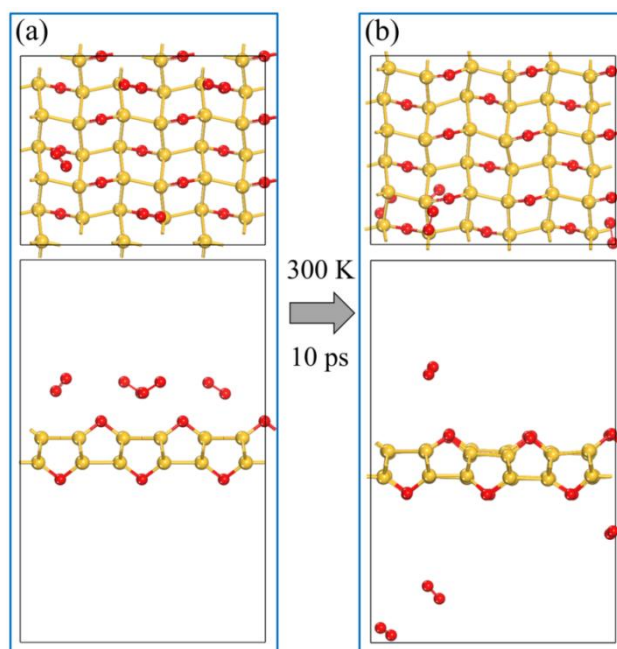


Figure S2. Top and side view of snapshots for the (a) initial and (b) final configurations of silicether exposed in O_2 molecules after 10 ps AIMD simulations with temperature at 300 K. The simulated cell contains a 3×3 silicether supercell and 4 O_2 molecules. The O_2 molecules under the lower surface arise from the O_2 molecules moving from one cell to another. It reveals a process that O_2 molecules move away from the silicether surface rather than through it.

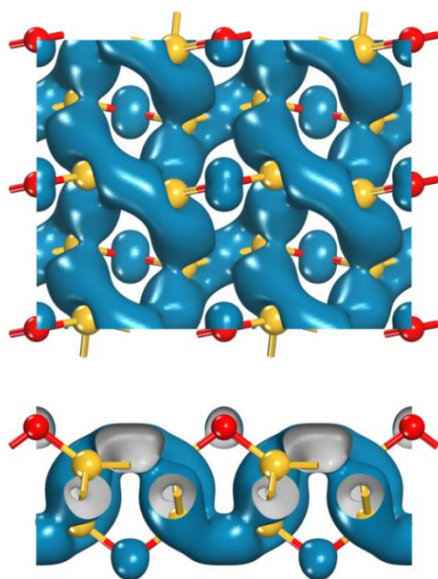


Figure S3. Top and side views of the band decomposed charge densities for VBM.

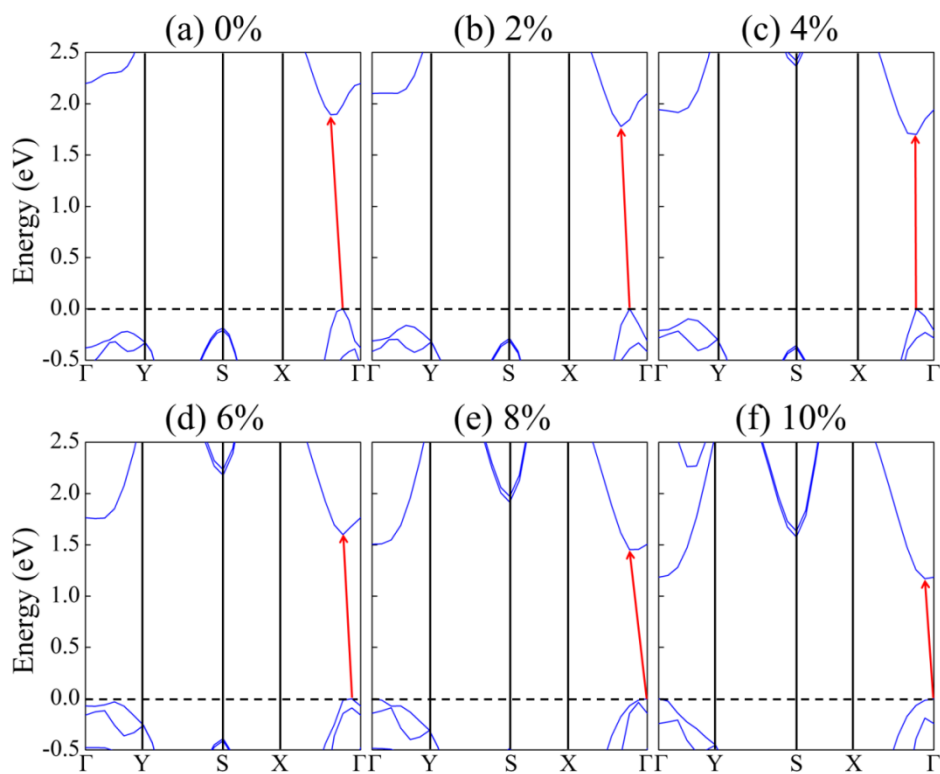


Figure S4. Band structures (HSE06) of silicether with respect to tensile strain along the armchair direction.

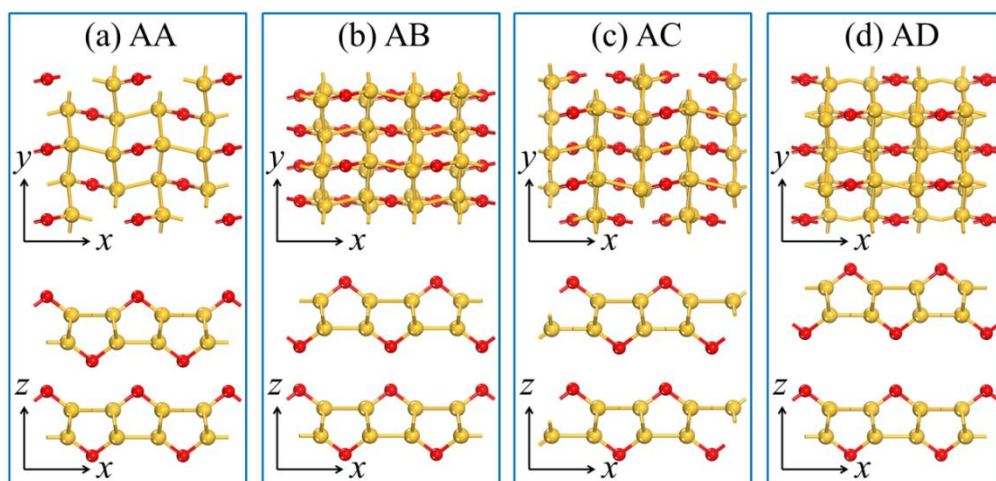


Figure S5. Top and side views of bilayer silicether for (a) AA, (b) AB, (c) AC, and (d) AD stacking patterns. AA: the top layer is directly stacked on the bottom layer; AB (AC): the upper layer of AA-stacking is shifted by half of a primitive cell along the x (y) direction; AD: the upper layer of AA-stacking is shifted by half of a primitive cell both along the x and along the y direction.

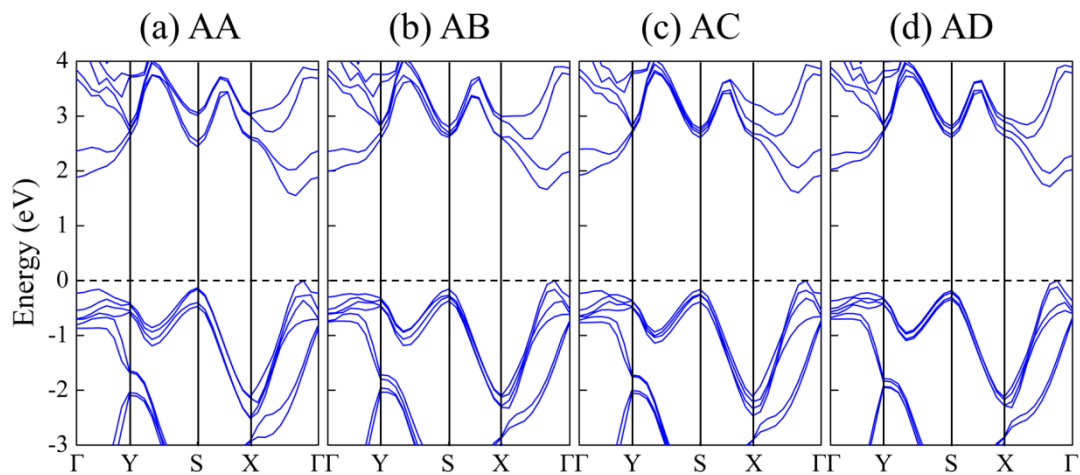


Figure S6. Band structures (HSE06) of bilayer silicether for (a) AA, (b) AB, (c) AC, and (d) AD stacking patterns.

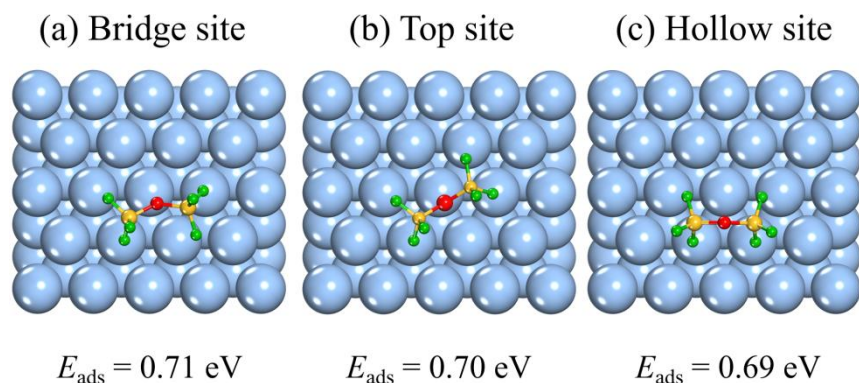


Figure S7. Three possible adsorption sites (bridge, top, and hollow) for disilyl ether adsorbed on Ag (100). The Ag(100) surface is modelled by a four-layered 4×4 orthogonal supercell, with the bottom two Ag layers fixed in their bulk positions during the geometry relaxation. The adsorption energy (E_{ads}) is given for each structure, defined as $E_{\text{ads}} = E_{\text{sub}} + E_{\text{dis}} - E_{\text{total}}$, where E_{sub} , E_{dis} , and E_{total} are the total energies of the pristine substrate, the disilyl ether molecule in gas phase, and the disilyl ether adsorbed substrate, respectively.

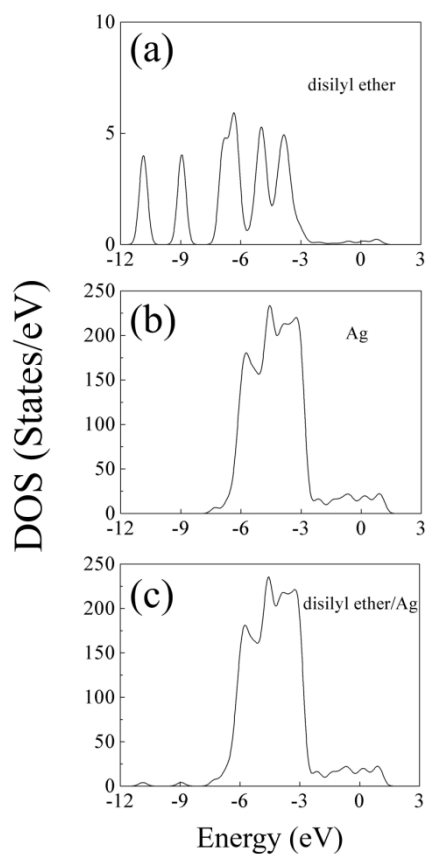


Figure S8. DOS of (a) disilyl ether, (b) Ag(100) substrate and (c) disilyl ether/Ag system.

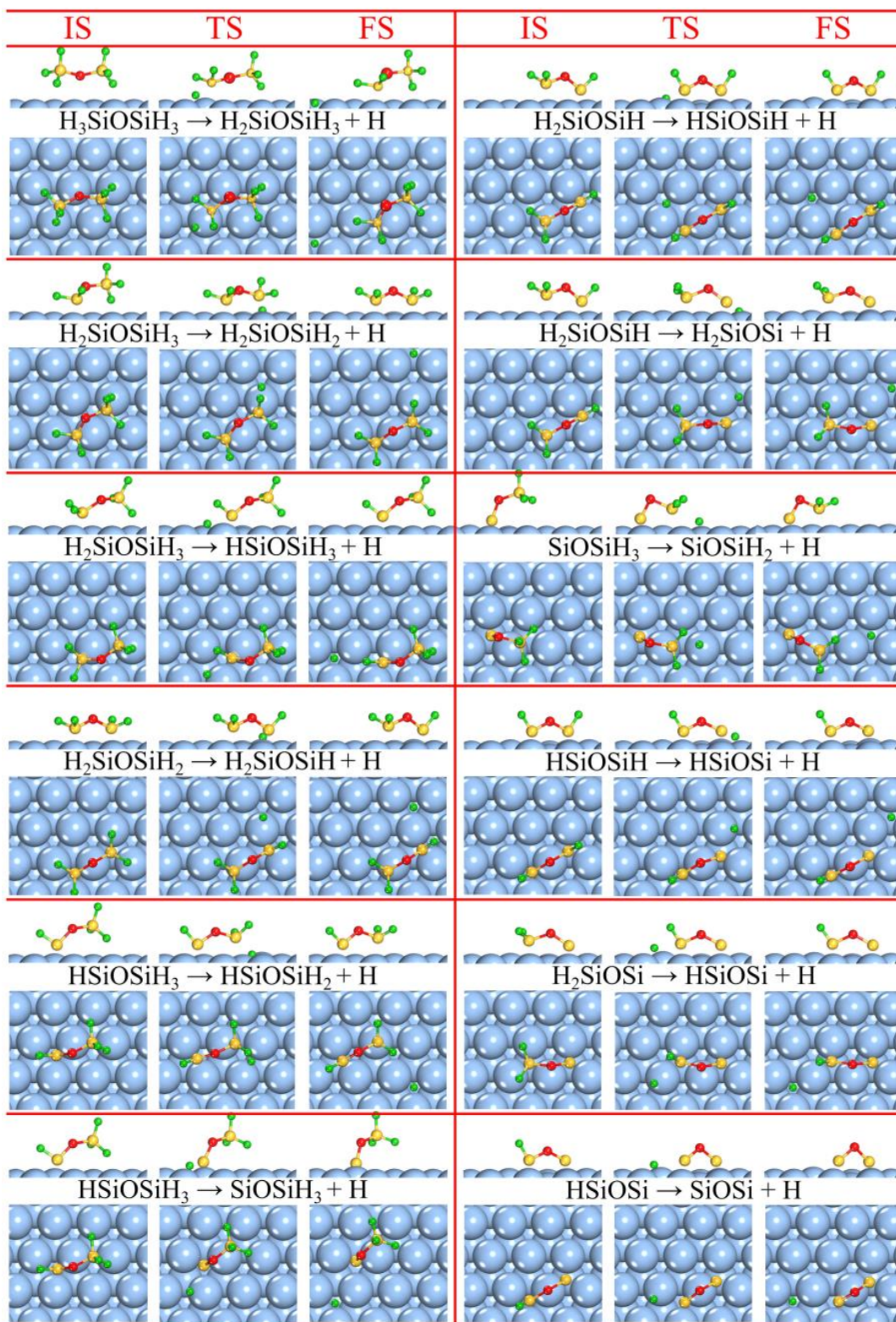


Figure S9. Geometric structures of the initial state (IS), transition state (TS), and final state (FS) of the every dehydrogenation step for disilyl ether on Ag (100).

Table S1. Structural informations of the silicether monolayer.

Structure	Space Group	Lattice	Wyckoff Positions (fractional)			
		Parameters	atoms	<i>x</i>	<i>y</i>	<i>z</i>
Silicether	<i>P2₁2₁2</i>	<i>a</i> =4.9400 Å	Si(4c)	0.7707	0.4317	0.4680
		<i>b</i> =3.8103 Å	O(2a)	0	0	0.5755
		<i>c</i> =23.1233 Å				
		$\alpha=\beta=\gamma=90^\circ$				

Computational Methods of Carrier Mobility

We estimate the carrier mobility for silicether at room temperature (300 K) by using

$$\mu_x \approx \frac{eh^3 \left(\frac{5C_x + 3C_y}{8} \right)}{k_B T m_x^{\frac{3}{2}} m_y^{\frac{1}{2}} \left(\frac{9E_{1x}^2 + 7E_{1x}E_{1y} + 4E_{1y}^2}{20} \right)},$$

where m_x is the effective mass

in the transport direction and m_y is the effective mass in another direction. The term E_1

defined by $E_1 = \frac{\Delta V}{(\Delta l/l_0)}$ represents the DP constant of the valence-band minimum

(VBM) for hole or the conduction-band maximum (CBM) for electron along the transport direction. Here, ΔV denotes the energy change of VBM or CBM when silicether

is compressed or dilated from the equilibrium l_0 by a distance of Δl . The term C_x (C_y) is the in-plane stiffness of the longitudinal strain in the x (y) direction, which can be derived

from $\frac{\Delta E}{S_0} = C_x \frac{(\Delta l/l_0)^2}{2}$. ΔE denotes the total energy difference under each strain, and S_0

is the lattice area of pristine silicether. We use $\Delta l/l_0$ ranging from -0.5% to 0.5% to fit the values of E_1 and C_{2D} (Fig. S10).

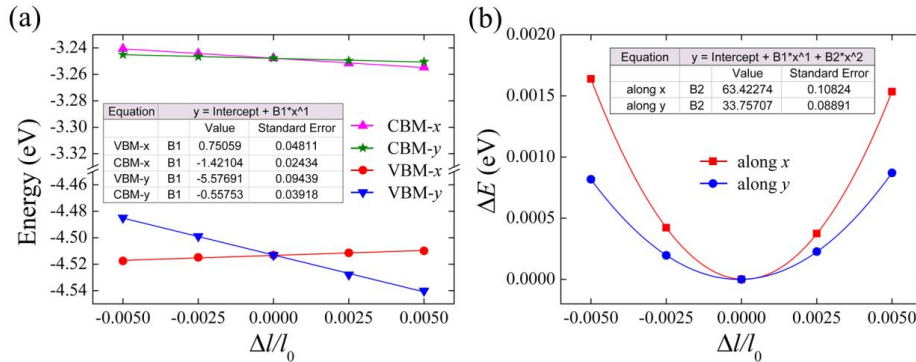


Figure S10. (a) DP constants and (b) in-plane stiffness of silicether along x and y directions at the PBE level of theory.