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Supplementary Materials: Theoretical Analysis of Si_2H_6 Adsorption on Hydrogenated Silicon Surfaces for Fast Deposition Using Intermediate Pressure SiH_4 Capacitively Coupled Plasma

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This supporting information provides details of the structures of the adsorption, transition, and reaction states of Si_2H_6 on H-50% covered Si(001) and Si(111) surfaces.

1. H-50% covered Si(001) and H-50% covered Si(111) surfaces

The adsorption energies of Si_2H_6 were calculated on two different Si surfaces for each geometry and position, and are summarized in Tables S1–S2.

2. Optimized structures

Figures S1–S4 show the optimized structures for specific reaction states, such as at the initial, transition, and final step for the decomposition of Si_2H_6 on the H-50% covered Si(001) and Si(111) surfaces. The energies of both the initial and final states of the Si, H, and Si_xH_y species remaining at the most stable sites on these surfaces were calculated for each geometry and at each position. Tables S3–S6 indicate the activation energies and reaction energies for the overall reactions of the Si_2H_6 decomposition on the above-mentioned two Si surfaces. These tables provide information on whether the Si_xH_y reaction is energetically stable or unstable for each reaction step.

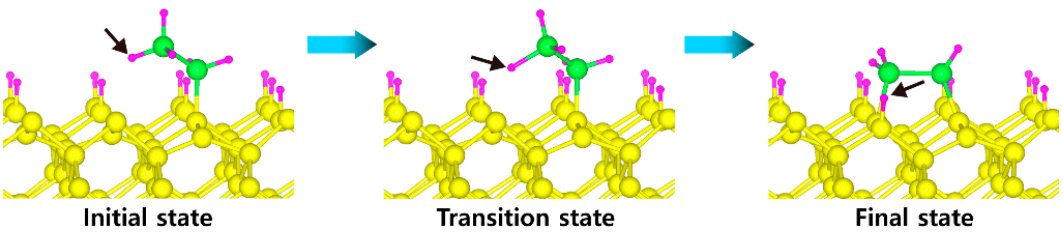
Table S1. Adsorption energies of Si_2H_6 on the H-50% covered Si(001)-(4 × 4) surface, calculated for each geometry and position.

Geometry	Position	E_{ads} (eV)
1	1	−0.35464
1	2	−0.35663
1	3	−0.34548
1	4	−0.25754
1	**5**	**−0.39696**
1	6	−0.34459
1	7	−0.27298
1	8	−0.32587
1	9	−0.25409
1	10	−0.24295
2	1	−0.19820
2	2	−0.22156
2	3	−0.24548
2	4	−0.20697
2	5	−0.17435
2	6	−0.27282
2	7	−0.15625
2	8	−0.20436
2	9	−0.20208
2	10	−0.18826

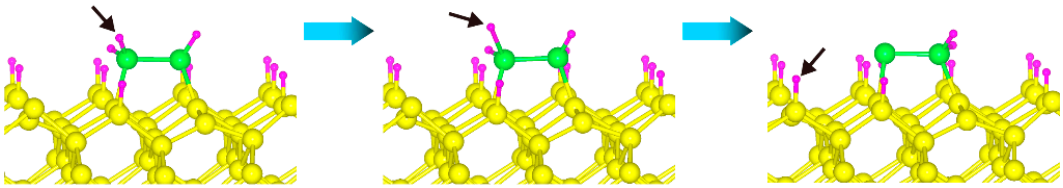
Table S2. Adsorption energies of Si_2H_6 on the H-50% covered Si(111)-(4 × 4) surface, calculated for each geometry and position.

Geometry	Position	E_{ads} (eV)
1	1	−0.26245
1	**2**	**−0.28634**
1	3	−0.26425
1	4	−0.25195
1	5	−0.21753
1	6	−0.23793
2	1	−0.24621
2	2	−0.20771
2	3	−0.27621
2	4	−0.22102
2	5	−0.22715
2	6	−0.21653

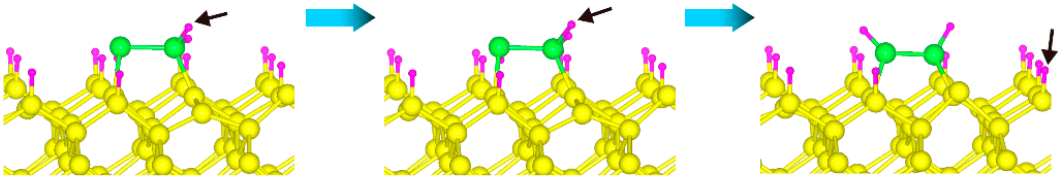
2nd reaction step : Si-H bond dissociation



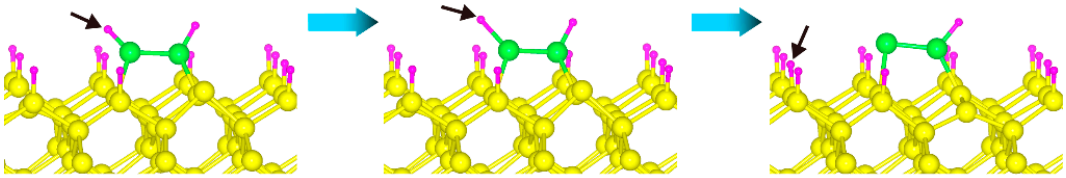
3rd reaction step : Si-H bond dissociation



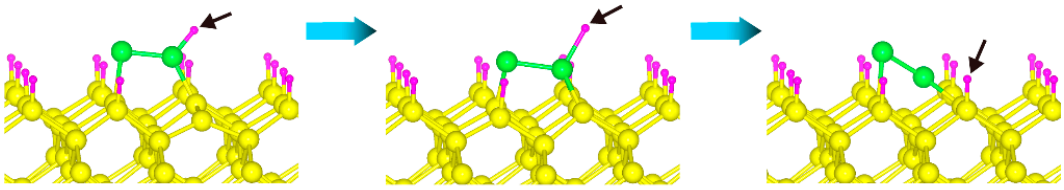
4th reaction step : Si-H bond dissociation



5th reaction step : Si-H bond dissociation



6th reaction step : Si-H bond dissociation



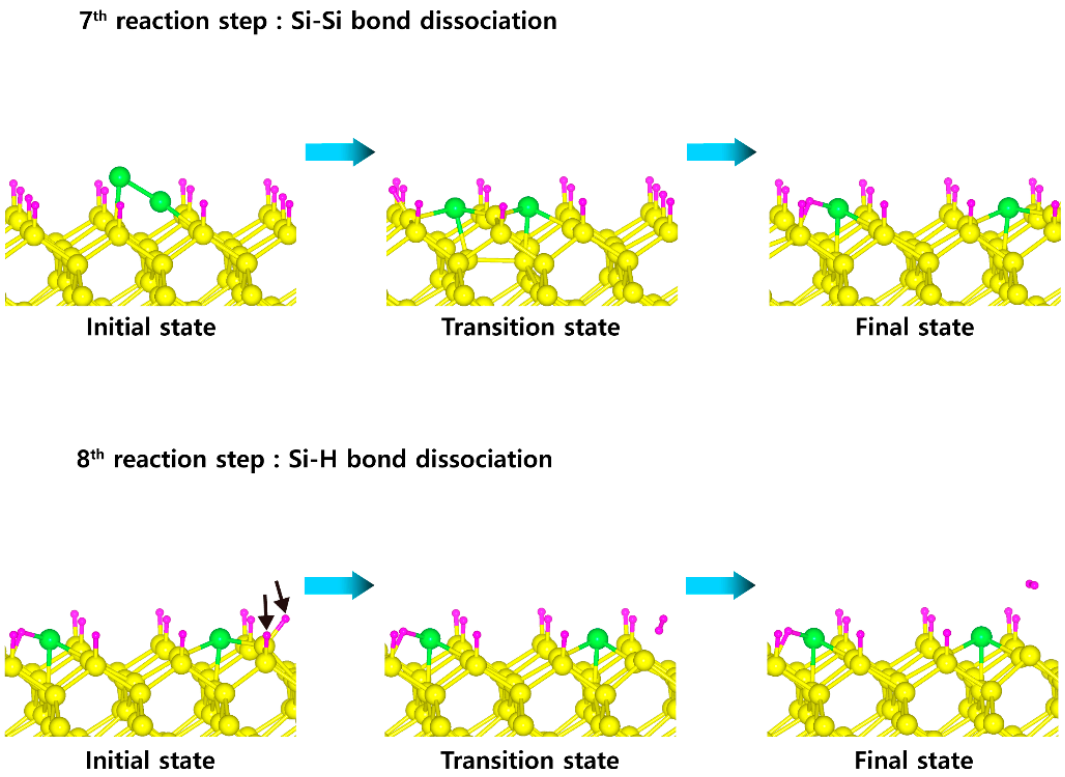
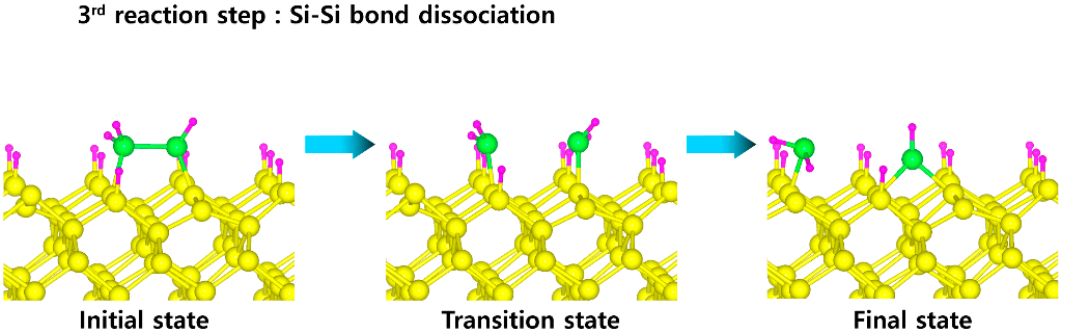


Figure S1. Initial (IS), transition (TS), and final (FS) states of intermediate reactions of Si_2H_6 from the 2nd reaction step to the 8th reaction step for path a on the H-50% covered Si(001) surface.

Table S3. Activation energies (E_a, eV) and reaction energies (E_{rxn}, eV) of Si_2H_6 dissociation for path a on the H-50% covered Si(001) surface.

Reaction step	Bond dissociation	E_a (eV)	E_{rxn} (eV)
Step 1	Si-H	0.15	−2.04
Step 2	Si-H	0.64	−1.97
Step 3	Si-H	1.51	0.57
Step 4	Si-H	0.99	−1.48
Step 5	Si-H	1.63	0.43
Step 6	Si-H	0.22	−0.09
Step 7	Si-Si	1.22	0.93
Step 8	Si-H	0.83	0.78



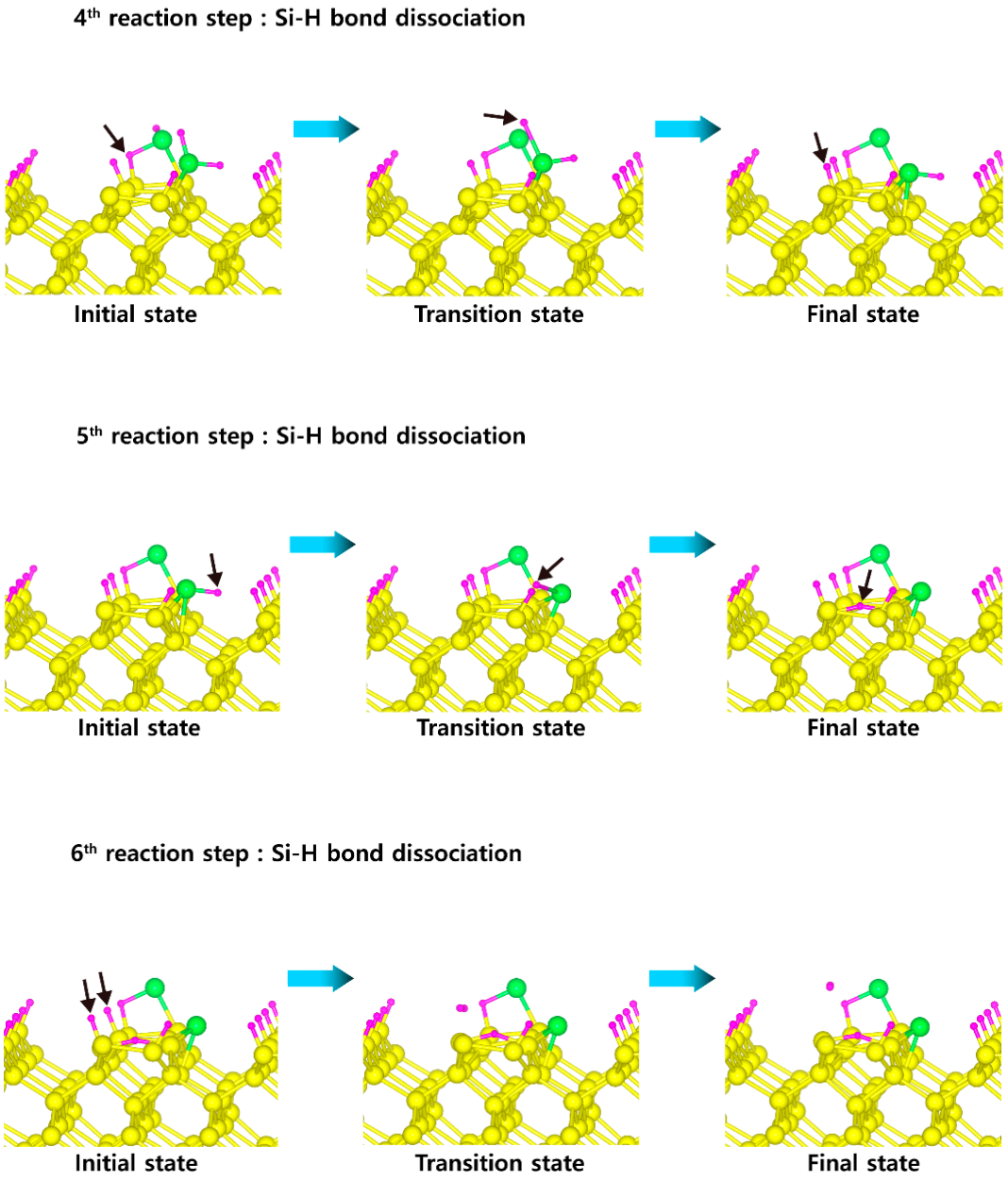
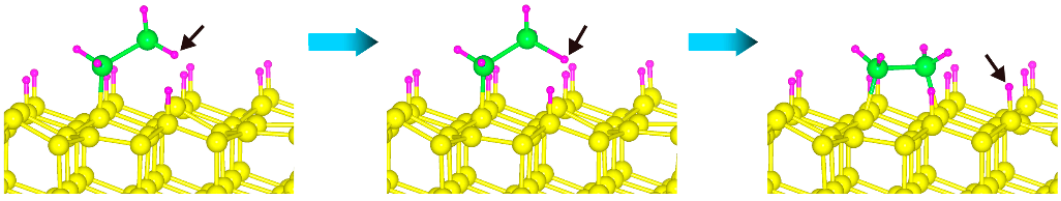


Figure S2. Initial (IS), transition (TS), and final (FS) states of intermediate reactions of Si_2H_6 from the 3rd reaction step to the 6th reaction step for path b on the H-50% covered Si(001) surface.

Table S4. Activation energies (E_a, eV) and reaction energies (E_{rxn}, eV) of Si_2H_6 dissociation for path b on the H-50% covered Si(001) surface.

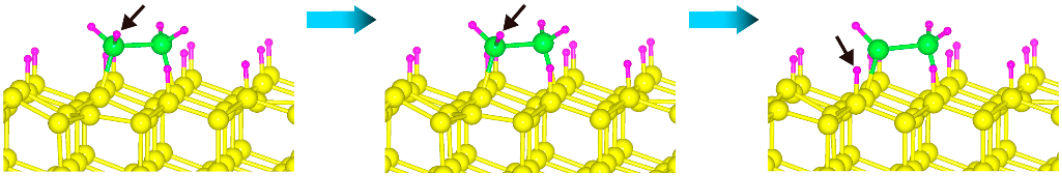
Reaction step	Bond dissociation	E_a (eV)	E_{rxn} (eV)
Step 3	Si-Si	2.52	0.69
Step 4	Si-H	1.15	−0.35
Step 5	Si-H	1.68	1.04
Step 6	Si-H	2.20	2.02

2nd reaction step : Si-H bond dissociation



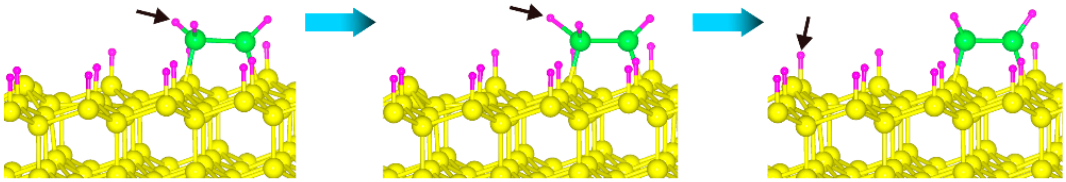
Initial state Transition state Final state

3rd reaction step : Si-H bond dissociation



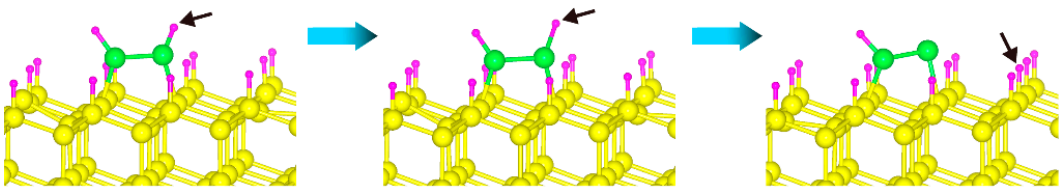
Initial state Transition state Final state

4th reaction step : Si-H bond dissociation



Initial state Transition state Final state

5th reaction step : Si-H bond dissociation



Initial state Transition state Final state

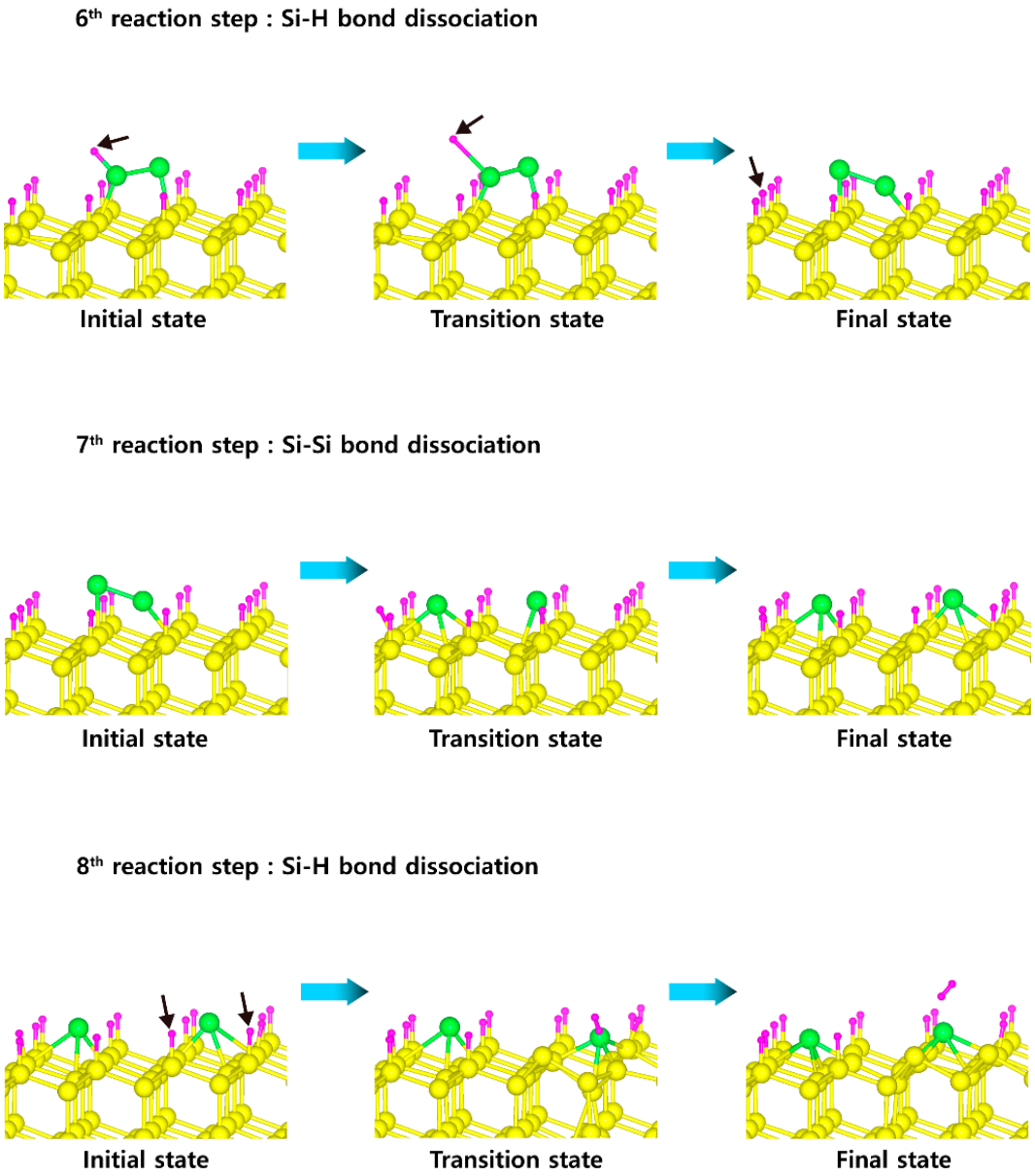


Figure S3. Initial (IS), transition (TS), and final (FS) states of intermediate reactions of Si_2H_6 from the 2nd reaction step to the 8th reaction step for path a on the H-50% covered Si(111) surface.

Table S5. Activation energies (E_a, eV) and reaction energies (E_{rxn}, eV) of Si_2H_6 dissociation for path a on the H-50% covered Si(111) surface.

Reaction step	Bond dissociation	E_a (eV)	E_{rxn} (eV)
Step 1	Si-H	0.22	−2.60
Step 2	Si-H	1.21	−2.29
Step 3	Si-H	1.31	0.40
Step 4	Si-H	0.94	−1.38
Step 5	Si-H	1.23	0.33
Step 6	Si-H	2.06	−0.12
Step 7	Si-Si	2.81	1.87
Step 8	Si-H	1.47	1.18

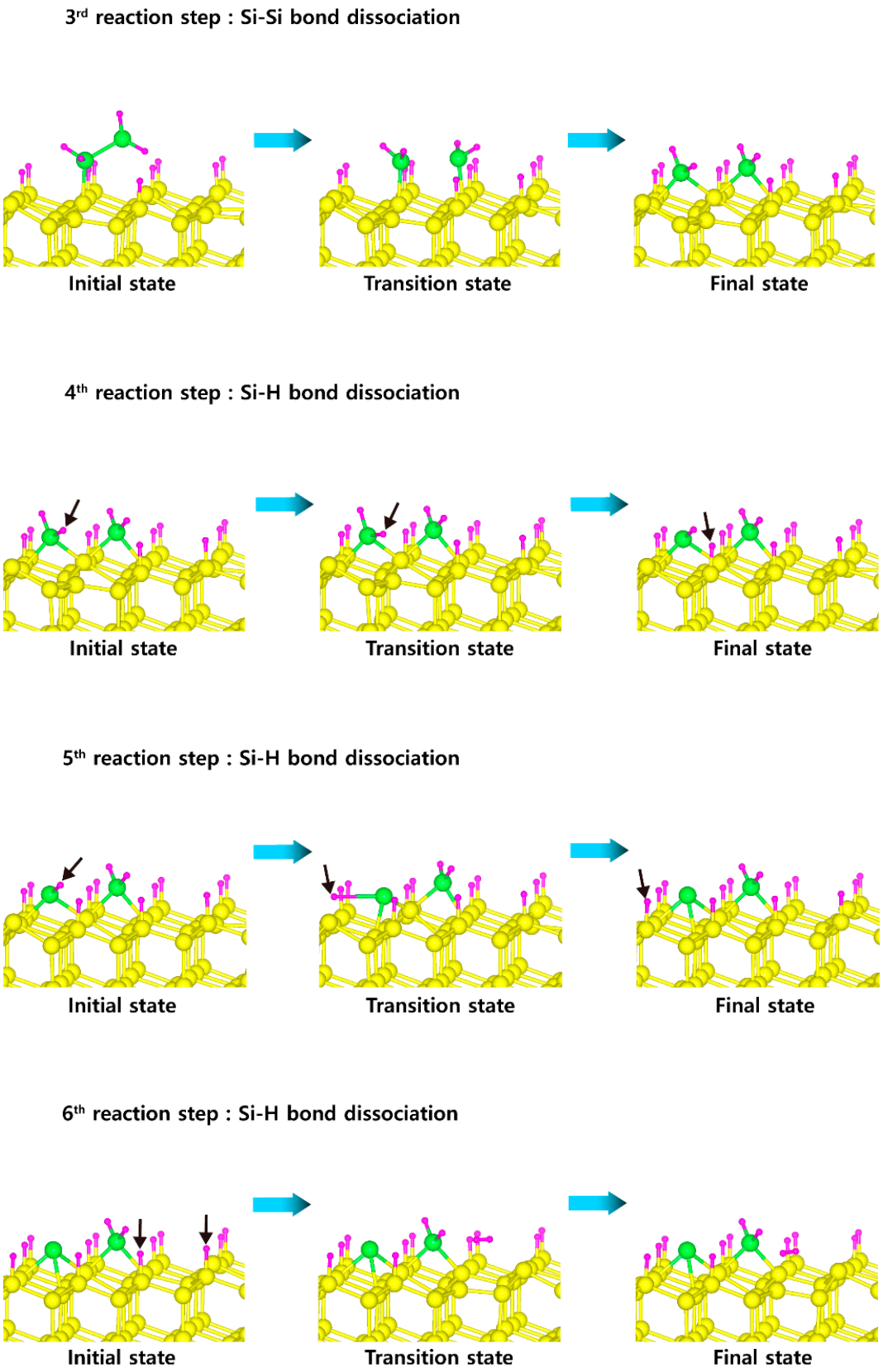


Figure S4. Initial (IS), transition (TS), and final (FS) states of intermediate reactions of Si_2H_6 from the 3rd reaction step to the 6th reaction step for path b on the H-50% covered Si(111) surface.

Table S6. Activation energies (E_a, eV) and reaction energies (E_{rxn}, eV) of Si_2H_6 dissociation for path b on the H-50% covered Si(111) surface.

Reaction step	Bond dissociation	E_a (eV)	E_{rxn} (eV)
Step 3	Si-Si	1.57	0.94
Step 4	Si-H	0.39	−0.52
Step 5	Si-H	0.43	−0.40
Step 6	Si-H	2.54	−0.29