Electronic Supplementary Information
On understanding trends of anisotropic alloying on Si(001) surface

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ENERGY BARRIERS USED IN KMC MODEL

We provide calculated energy barriers associated with possible atomic configurations in Table S1 and Table S2. These values are subsequently used during KMC modeling for hopping rate evaluation. We study transition energy barriers between two nearest adsorption minima in the directions parallel and perpendicular to SDRs for free and nucleated adatoms, where the later complex configurations are shown, for clarity, in Figure S1 and Figure S2. Configuration ordering in Tables is consistent with subfigure captions. Due to physical limits, we neglect more complex configurations and set the hopping rate to zero, if the configuration is considered stable. The details of nucleation process are given in the *Nucleation* paragraph in Section **2.2 Kinetic Monte-Carlo** in the Main text.

TABLE S1: Transition barriers for In atom

#	Configuration	$E_{\parallel}$, eV	$E_{\perp}$, eV
01	In free	0.260	0.241
02	In mon. + C-def	0.279	0.587
03	In dim. + C-def	0.468	0.445
04	In odd sized chain	0.357	0.697
05	In even sized chain	0.842	1.028
06	In homogeneous dim.	0.457	0.784
07	In mon. + 1 Ag	0.465	0.172
08	In mon. + 2 Ag	0.353	0.302
09	In dim. + C-def + 1 Ag	0.875	—
10	In odd-sized chain + 1 Ag	0.745	—
11	In even-sized chain + 1 Ag	0.853	—
12	In dim. + 1 Ag	0.609	—

TABLE S2: Transition barriers for Ag atoms

#	Configuration	$E_{\parallel}$, eV	$E_{\perp}$, eV
13	Ag free	0.887	0.639
14	Ag + C-def	1.053	0.831
15	Ag + 1 $Ag_{\perp}$	0.350	0.629
16	Ag + 2 $Ag_{\perp}$	0.319	—
17	Ag + 1 In mon.	0.945	0.615
18	Ag + 2 In mon.	0.971	—
19	Ag + 1 In dim.	1.015	0.721
20	Ag + 2 In dim.	0.9	—
21	Ag + 1 In mon. + C-def	1.466	—
22	Ag + 1 In dim. + C-def	0.806	—
23	Ag + 1 $Ag_{\perp}$ + C-def	1.036	—
24	Ag + 1 In mon. + 1 In dim.	1.326	—
25	Ag + 1 $Ag_{\perp}$ + 1 In mon.	0.551	—
26	Ag + 1 $Ag_{\perp}$ + 1 In dim.	0.691	—
27	Ag + 1 $Ag_{\parallel}$	0.434	0.65
28	Ag + 1 $Ag_{\parallel}$ + C-def	1.239	0.963
29	Ag + 1 $Ag_{\parallel}$ + 1 $Ag_{\perp}$	0.672	0.725
30	Ag + 1 $Ag_{\parallel}$ + 2 $Ag_{\perp}$	1.341	—
31	Ag + 1 $Ag_{\parallel}$ + 1 In mon.	1.102	-0.777
32	Ag + 1 $Ag_{\parallel}$ + 2 In mon.	0.846	—
33	Ag + 1 $Ag_{\parallel}$ + 1 In dim.	1.232	0.801
34	Ag + 1 $Ag_{\parallel}$ + 2 In dim.	1.445	—
35	Ag + 1 $Ag_{\parallel}$ + 1 In mon. + C-def	0.491	—
36	Ag + 1 $Ag_{\parallel}$ + 1 In dim. + C-def	0.608	—
37	Ag + 1 $Ag_{\parallel}$ + 1 $Ag_{\perp}$ + C-def	0.522	—
38	Ag + 1 $Ag_{\parallel}$ + 1 In mon. + 1 In dim.	1.338	—
39	Ag + 1 $Ag_{\parallel}$ + 1 $Ag_{\perp}$ + 1 In mon.	1.131	—
40	Ag + 1 $Ag_{\parallel}$ + 1 $Ag_{\perp}$ + 1 In dim.	1.252	—
41	Ag + 2 $Ag_{\parallel}$	—	0.888
42	Ag + 2 $Ag_{\parallel}$ + 1 In mon.	—	1.08
43	Ag + 2 $Ag_{\parallel}$ + 1 In dim.	—	0.927
44	Ag + 2 $Ag_{\parallel}$ + 1 $Ag_{\perp}$	—	0.661
45	Ag + 2 $Ag_{\parallel}$ + C-def	—	0.577
46	Ag dim. free (dimer diffusion)	0.273	0.538
47	Ag dim. free (dimer decay)	0.261	0.602
48	Ag dim. + 1 $Ag_{\perp}$ (dimer diffusion)	—	0.726
49	Ag dim. + 1 $Ag_{\perp}$ (dimer decay)	0.528	0.466
50	Ag dim. + 1 Ag. $dim_{\perp}$ (dimer decay)	0.314	0.488
51	Ag dim. + 1 In mon. (dimer decay)	0.176	0.273
52	Ag dim. + 1 In dim. (dimer diffusion)	0.666	1.958
53	Ag dim. + C-def (dimer decay)	0.146	0.250

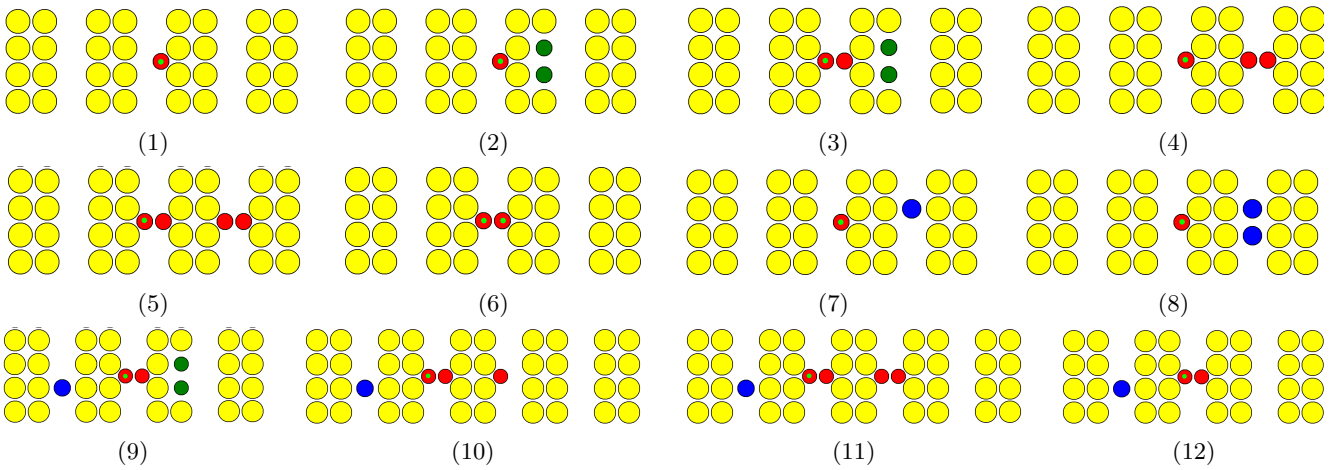

FIG. S1: Configurations attributed to atomic arrangements in Table S1. Indium atom transferring to the adjacent allowed site is highlighted by green dot. The subfigures numbering meets the configuration ordering in Table S1. The red and blue circles depict In and Ag adatoms, the SDRs are introduced by yellow circles, the C-defects are highlighted by green circles.

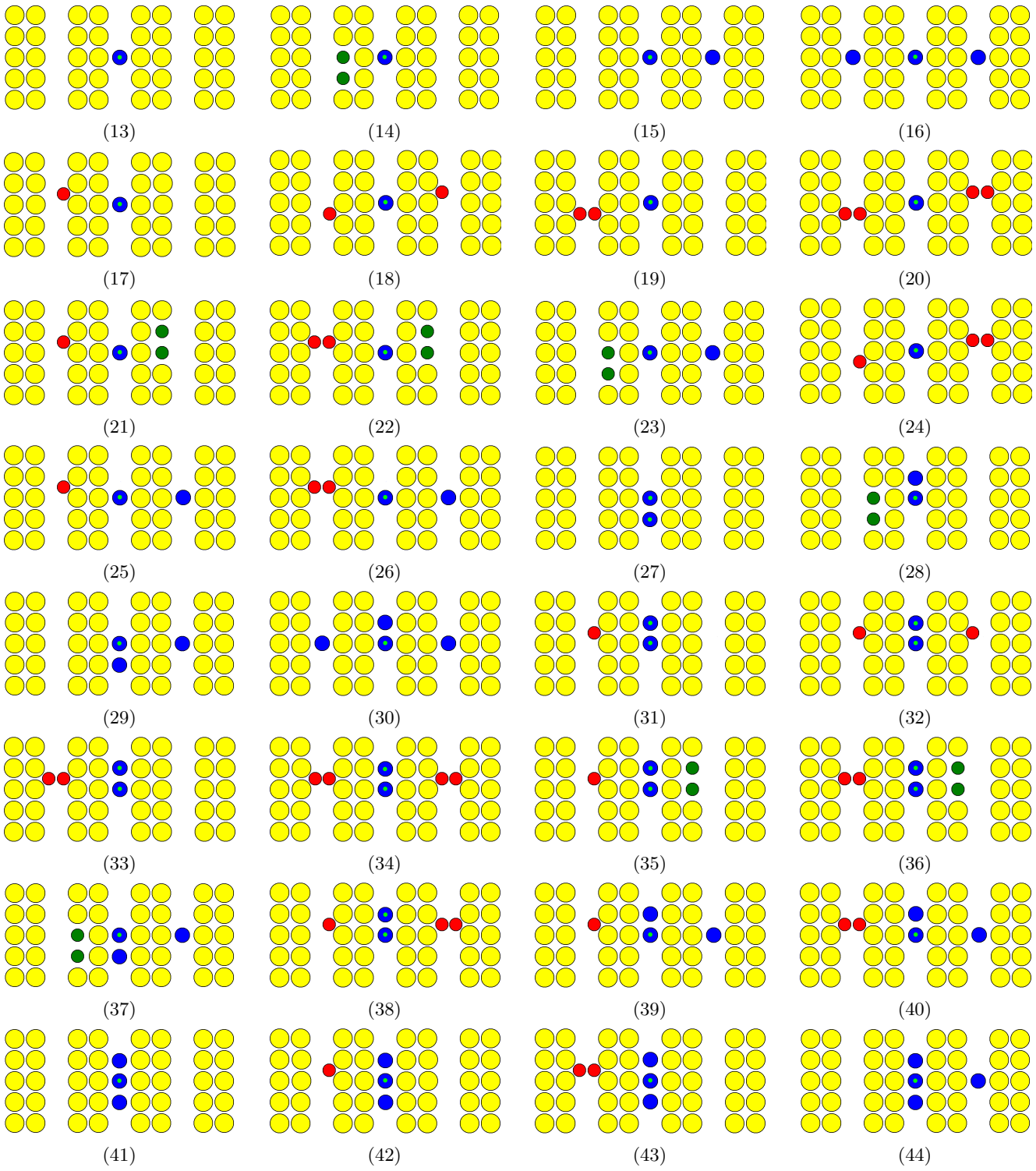

FIG. S2: Atomic configurations given in Table S2. Ag adatom moving between two nearest adsorption minima is marked with green dot. The subfigures numbering matches the configuration ordering in Table S2. The red and blue circles depict In and Ag adatoms, the SDRs are introduced by yellow circles, the C-defects are highlighted by green circles. The figure continues on the following page.

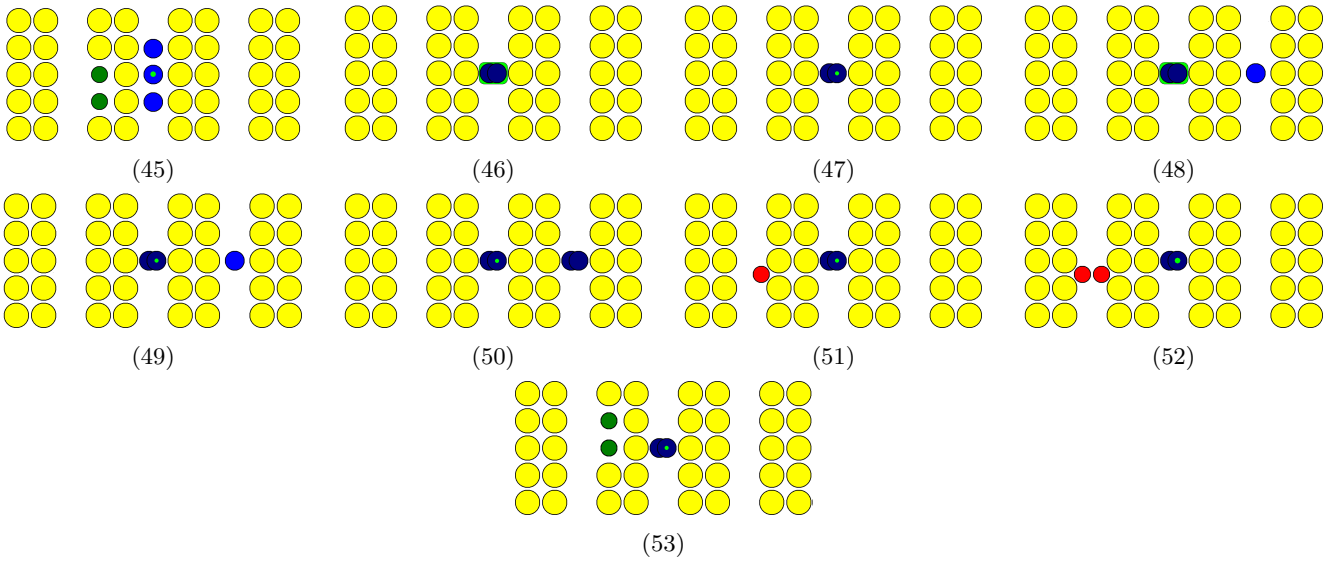

FIG. S2: Atomic configurations given in Table S2. The black oval represents Ag dimer configuration. Ag adatom moving between two nearest adsorption minima is marked with green dot. Configurations 46 and 48 refer to dimer diffusion. The subfigures numbering matches the configuration ordering in Table S2. The figure starts on the previous page.

FULL SNAPSHOT OF AG-IN ARRANGEMENT ON SILICON SURFACE CALCULATED WITHIN KMC APPROACH

Here we show a full snapshots of Ag-In ordering found using developed formalism, where the lattice size is (100×201), the C-defect density is 0.006, the temperature is $T = 300$ K, the coverage θ is 0.1 ML, and the Ag:In ratio is 1:1 (Figure S3).

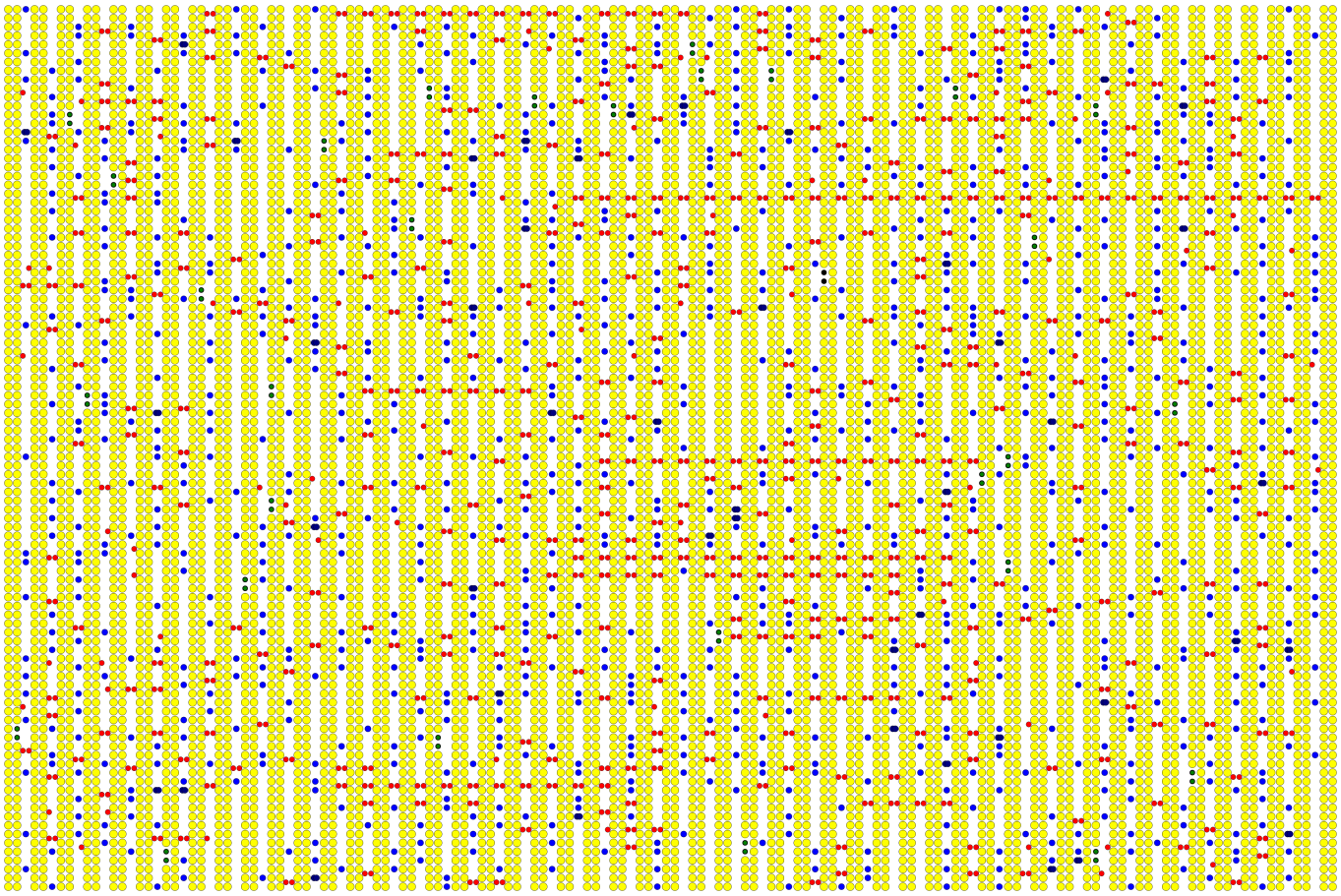

FIG. S3: Full snapshot of Ag-In configuration obtained using KMC simulation at the coverage $\theta = 0.1$ ML, the C-defect density is 0.006, the temperature is $T = 300$ K. The red and blue circles depict In and Ag adatoms, respectively. The silicon atoms attributed to SDRs are indicated by yellow circles. Ag dimers are represented by black ovals, while the C-defects are highlighed by green circles

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