Ab Initio Study of H_2 Associative Desorption on Ad-Dimer Reconstructed Si(001) and Ge(001)-(2×1) Surfaces

R. C. Longo,[*,†] J. H. G. Owen,[*,‡] S. McDonnell,[†] J. B. Ballard,[‡] R. M. Wallace,[†] J. N. Randall,[*,‡] Y. J. Chabal,[†] and K. Cho[*,†]

Department of Materials Science & Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA, and Zyvex Labs, LLC, 1301 N. Plano rd., Richardson, Texas 75081, USA

E-mail: roberto.longo@utdallas.edu; jowen@zyvexlabs.com; jrandall@zyvexlabs.com; kjcho@utdallas.edu

[*]To whom correspondence should be addressed

[†]Department of Materials Science & Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA

[‡]Zyvex Labs, LLC, 1301 N. Plano rd., Richardson, Texas 75081, USA

Table 1: Electronic band gaps (in eV) of the ad-dimer reconstructed Si(001)-(2x1) and Ge(001)-(2x1) surfaces (with 6 H atoms) and after the 1^{st} step of the three H_2 desorption pathways considered in this work (with 4 H atoms), as obtained with the HSE06 functional (the values obtained with GGA are shown in parentheses).

System	6 H	4 H (Pathway 1)	4 H (Pathway 2)	4 H (Pathway 3)
Si/Si(001)	1.15 (0.59)	1.12 (0.44)	1.07 (0.27)	0.56 (0.28)
Ge/Si(001)	1.25 (0.68)	1.22 (0.66)	1.18 (0.66)	0.59 (0.26)
Si/Ge(001)	1.02 (0.39)	0.97 (0.29)	0.99 (0.21)	0.86 (0.27)
Ge/Ge(001)	1.01 (0.49)	0.98 (0.47)	0.95 (0.47)	0.86 (0.42)

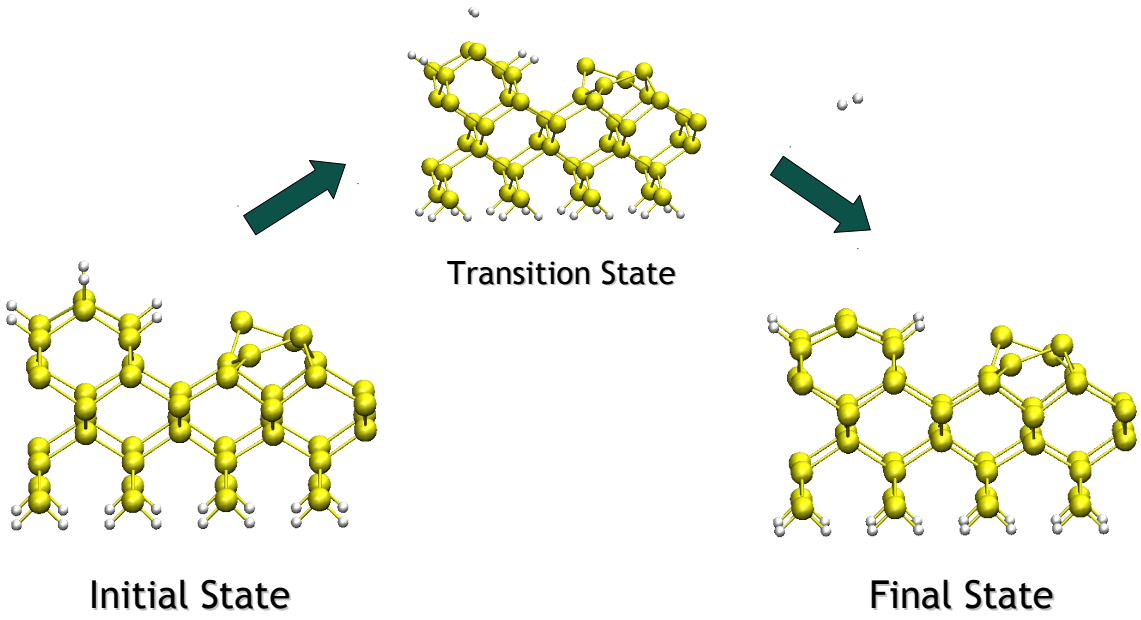

Figure 1: Lateral view of the initial, transition state and final configurations of a typical 1^{st} step of the H_2 desorption process from Si or Ge ad-dimers on the Si(001)-(2x1) or Ge(001)-(2x1) surfaces.

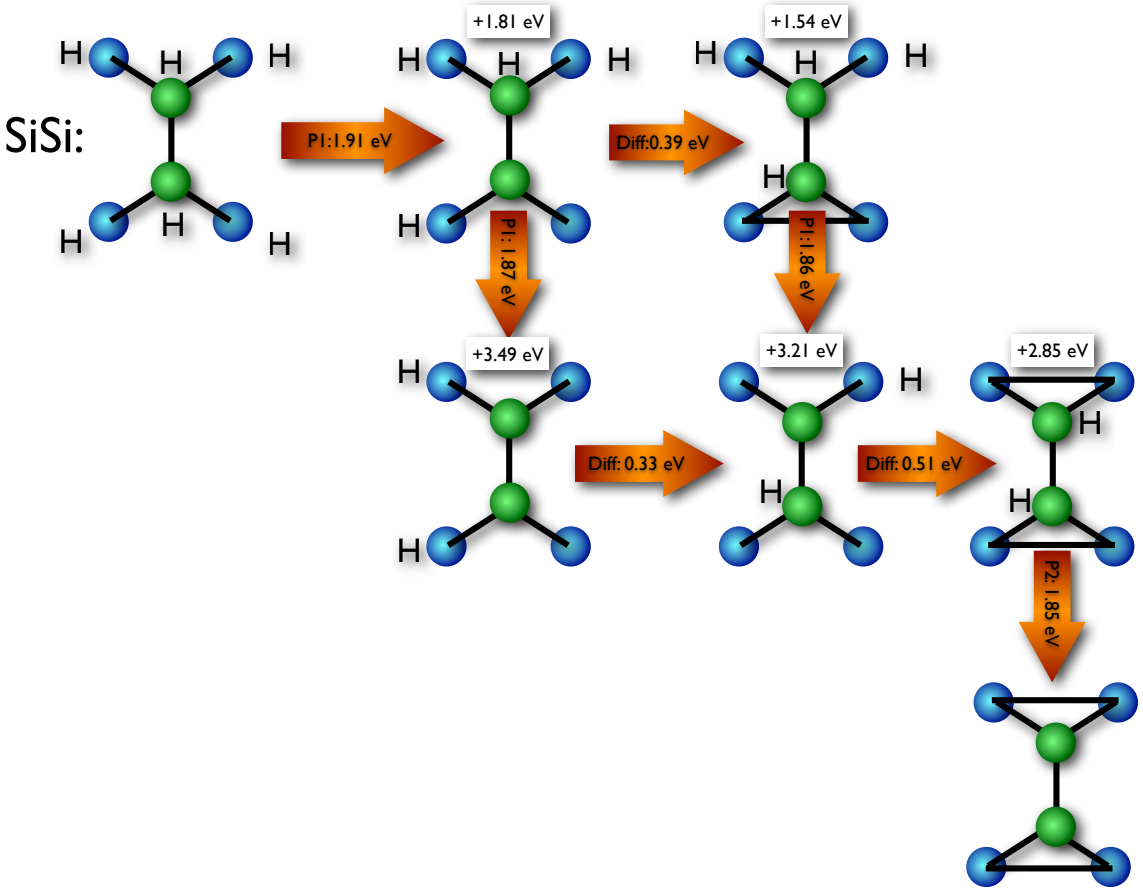

Figure 2: Most likely desorption paths followed during the H_2 desorption process from Si addimers on the Si(001)-(2x1) surface. The numbers on the arrows show the corresponding E_{des} kinetic barriers, either for H_2 desorption or diffusion. The numbers above the different configurations show the corresponding reaction energies, E_{rxn}. The kinetic barriers (E_{des}) are always referred to the previous configuration but, to allow a better understanding of the overall process, the reaction energies (E_{rxn}) are always referred to the initial energies (precursor adsorbed on the surface).

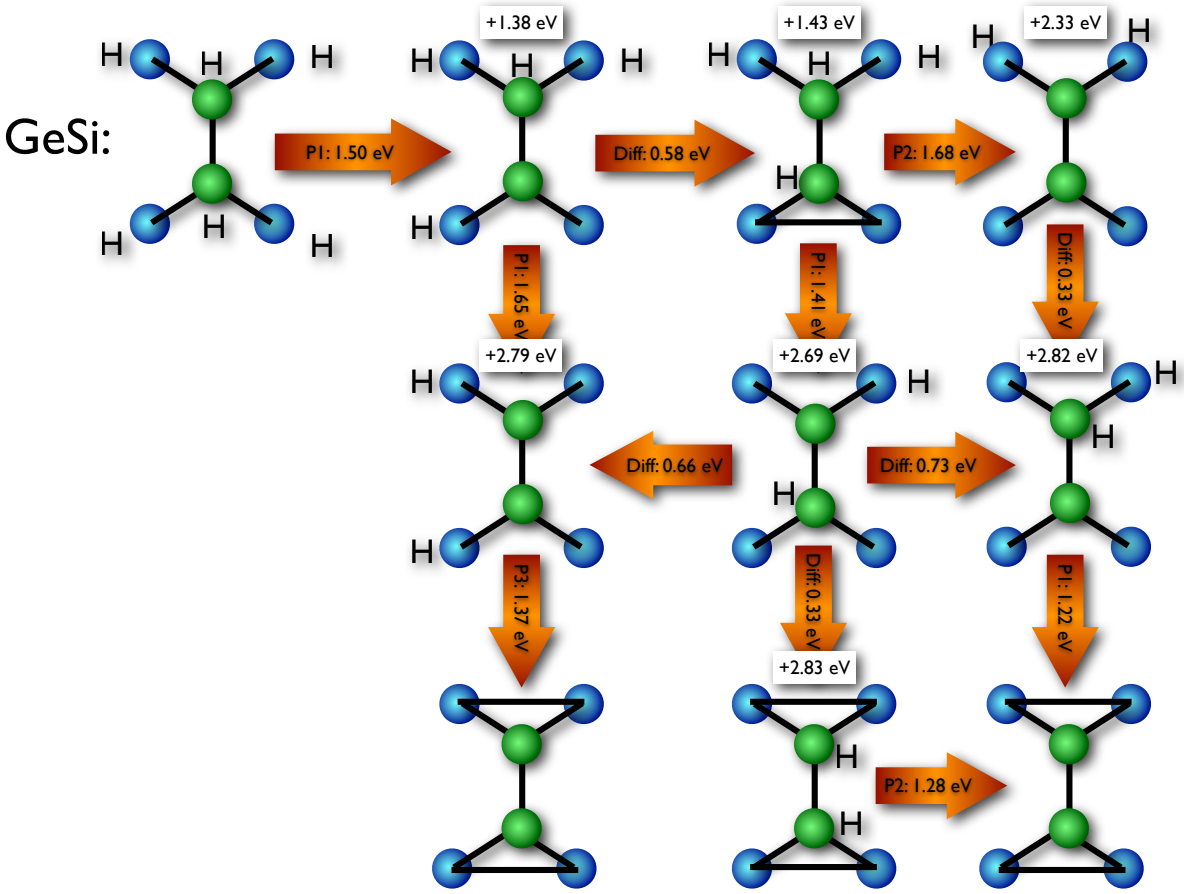

Figure 3: As for Fig. S1, but for Ge ad-dimers on the Si(001)-(2x1) surface.

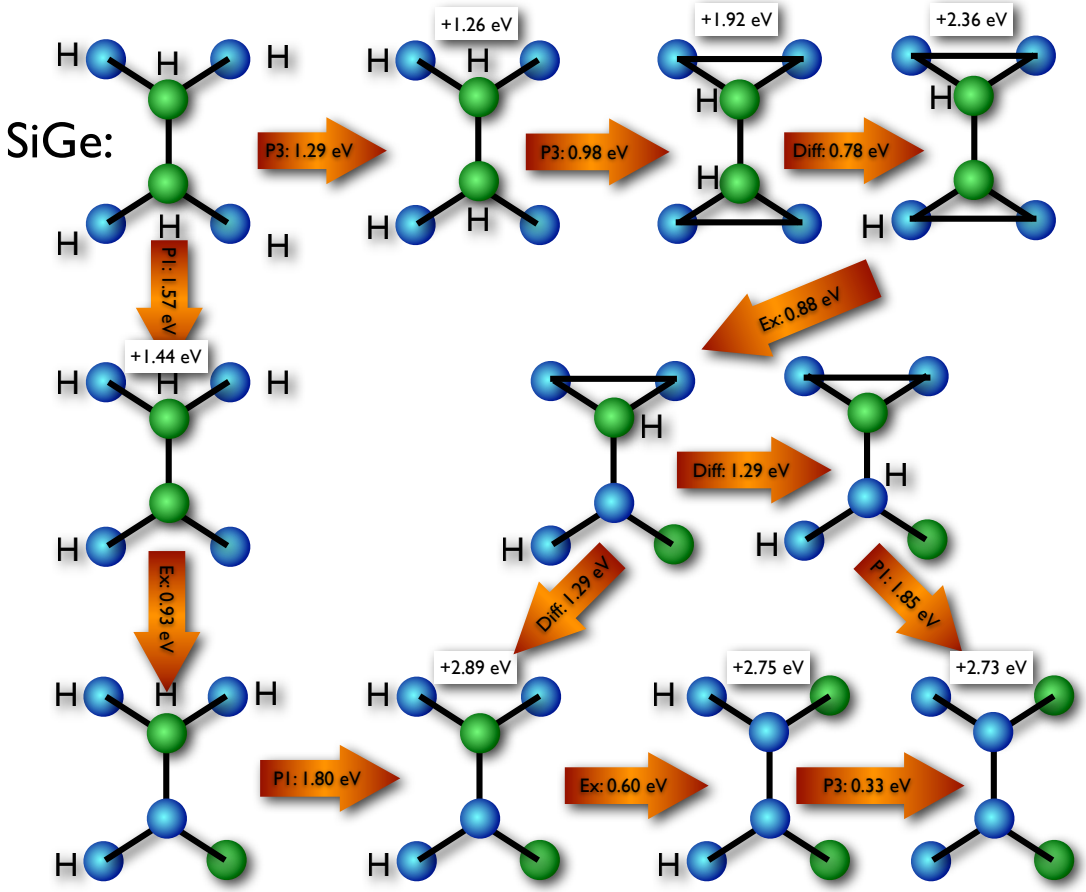

Figure 4: As for Fig. S1, but for Si ad-dimers on the Ge(001)-(2x1) surface.

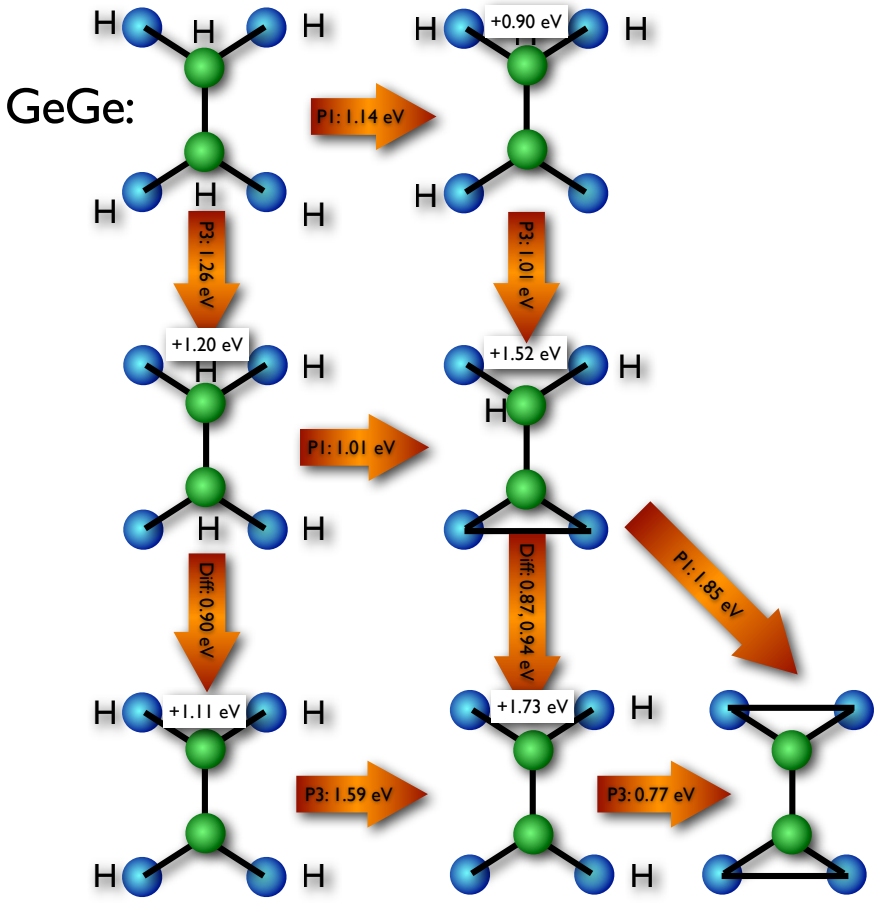

Figure 5: As for Fig. S1, but for Ge ad-dimers on the Ge(001)-(2x1) surface.