**Supporting Information**

Extraordinarily large kinetic isotope effect on

alkene hydrogenation over

Rh-based intermetallic compounds

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Table S1. Adsorption (*E*ad) and dissociation (*E*dis) energies of H2 on Rh-based surfaces.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | *E*ad (eV) | | *E*dis (eV) | |
| H2 | D2 | H2 | D2 |
| Rh | −0.049 | −0.049 | 0.013 | 0.011 |
| RhIn | −0.028 | −0.029 | 0.076 | 0.074 |
| RhPb2 | −0.046 | −0.049 | 0 | 0 |

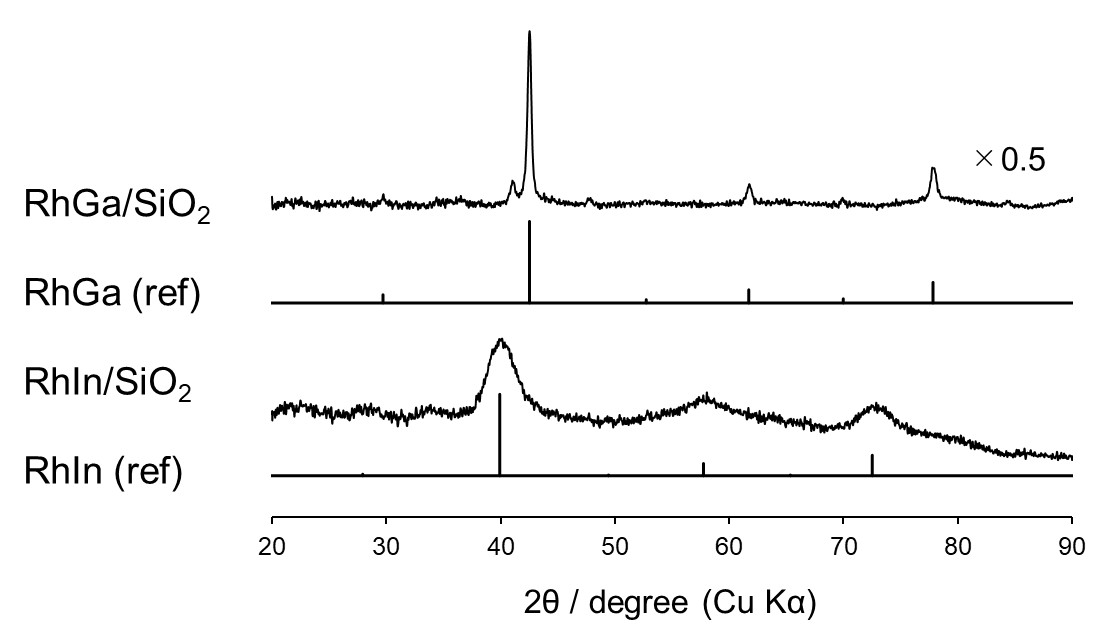


Figure S1. XRD patterns of RhGa/SiO2 and RhIn/SiO2. References are shown as black vertical lines. The desired intermetallic phases were observed with high phase purities.

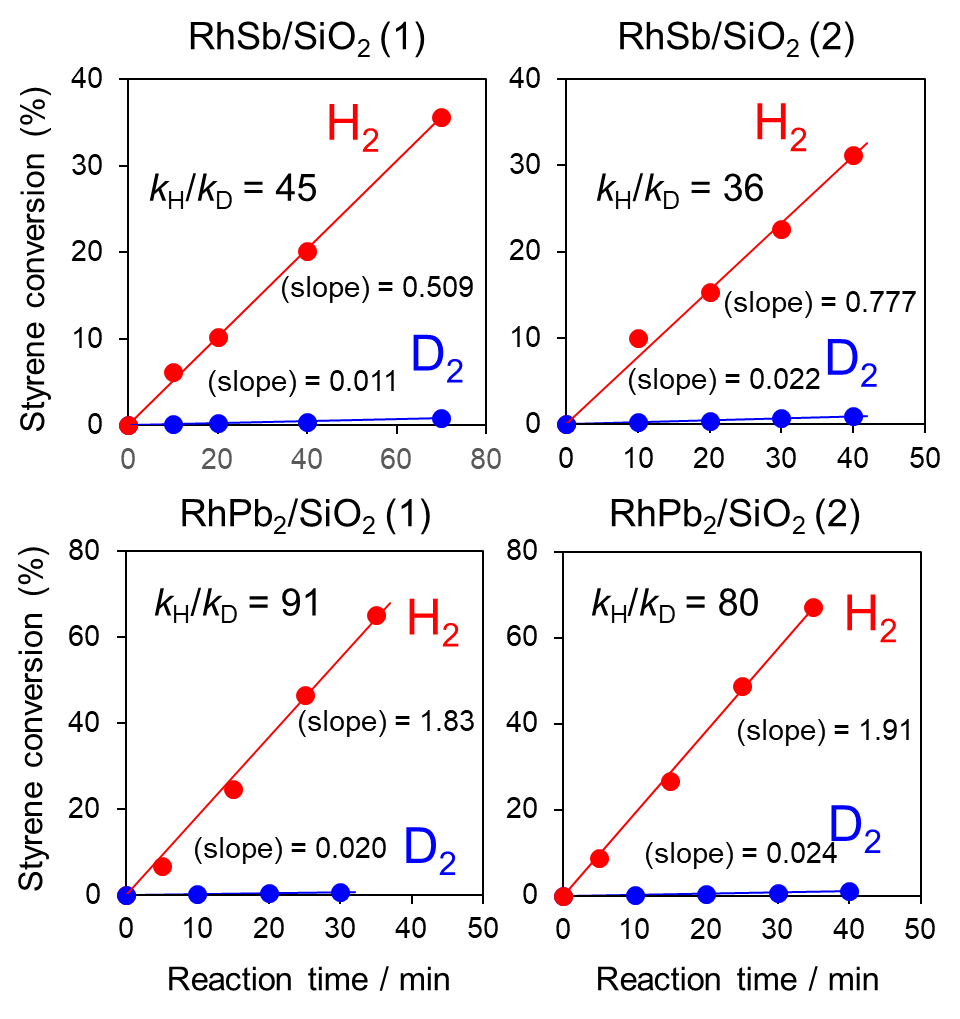


Figure S2. Time-course of styrene conversion in styrene hydrogenation over RhSb/SiO2 and RhPb2/SiO2 catalysts when H2 (red) or D2 (blue) was used as a hydrogen source.

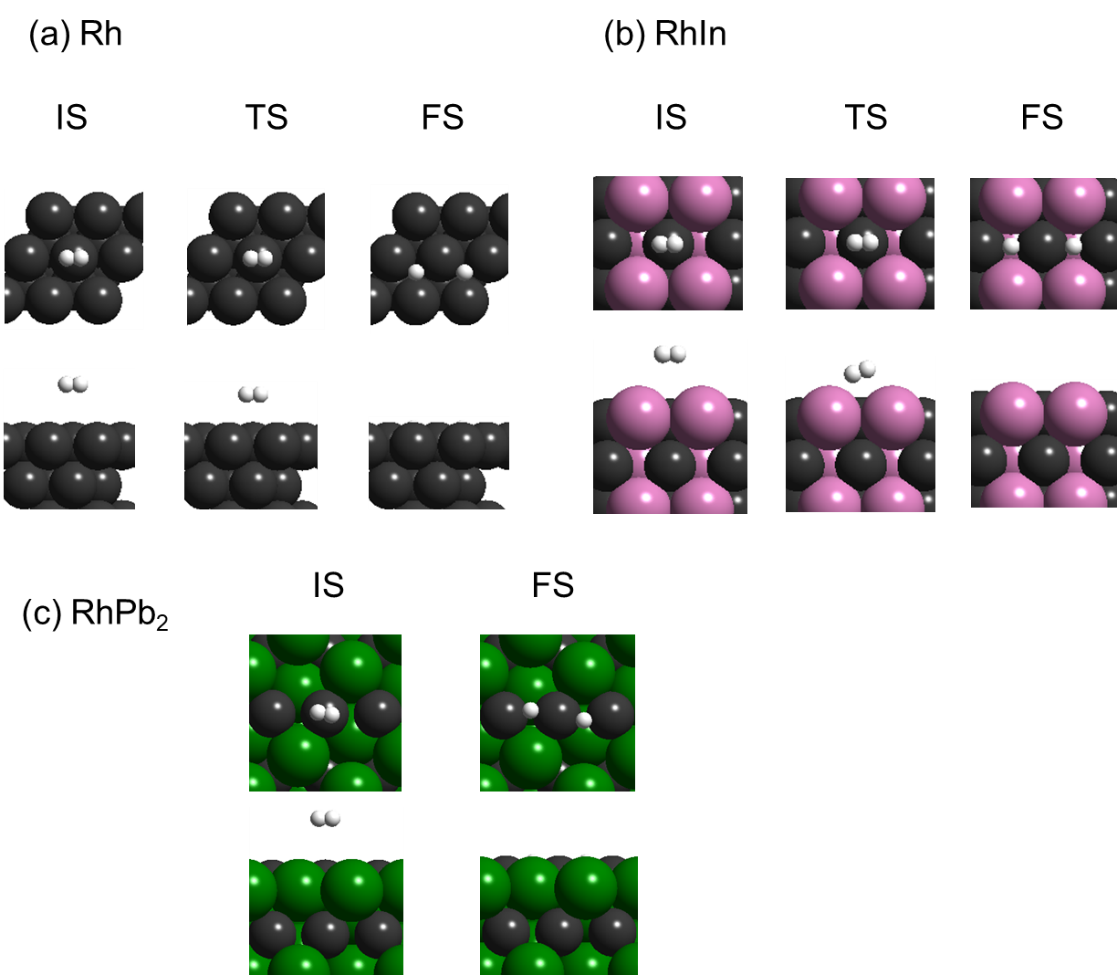


Figure S3. Structures of initial (IS: H2 molecule), transition (TS), and final (FS: two H atoms) states during H2 activation process over (a) Rh(111), (b) RhIn(110), and (c) RhPb2(100) surfaces.

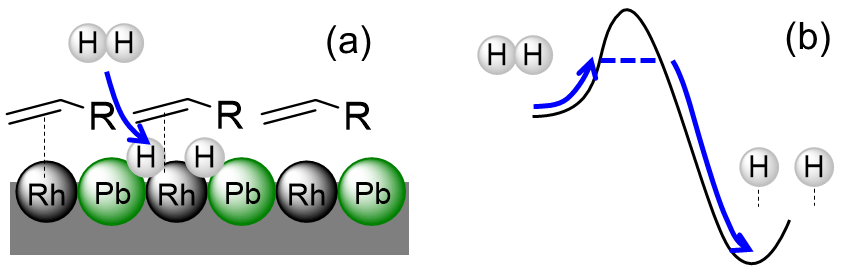


Figure S4. (a) Schematic illustration and (b) energy diagram of hydrogen dissociative adsorption on RhPb2 covered with alkene. The dotted line in (a) indicates adsorption of the C=C moiety on the Rh site.