Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Catalytic Modification in Dehydrogenation Properties of $KSiH_3$ (Electronic Supplementary Information)

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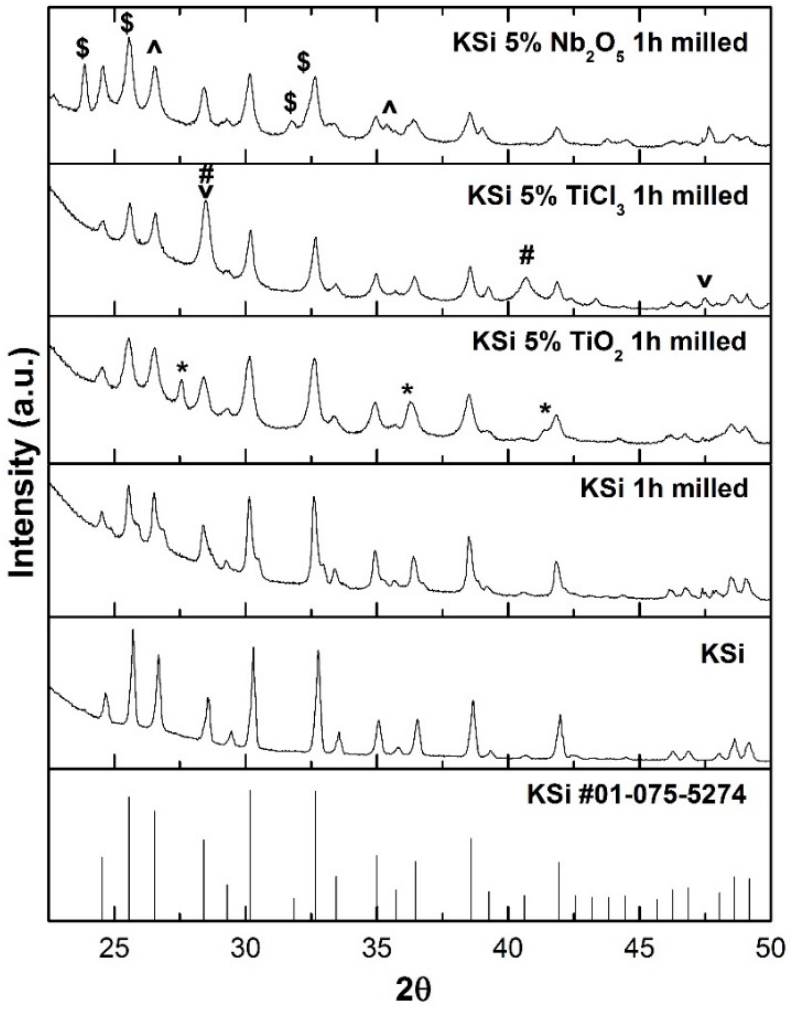

Fig. 1 XRD pattern of pristine and milled KSi with / without catalysts. Different phases are indexed by symbols (shown in brackets) as follows: TiO_2 # 01-084-1284 (*); KCl # 00-004-0587 (#); Nb_2O_5 # 00-019-0862 ($); NbO_2 # 01-071-4836 (^); Si # 01-080-0018 (v).

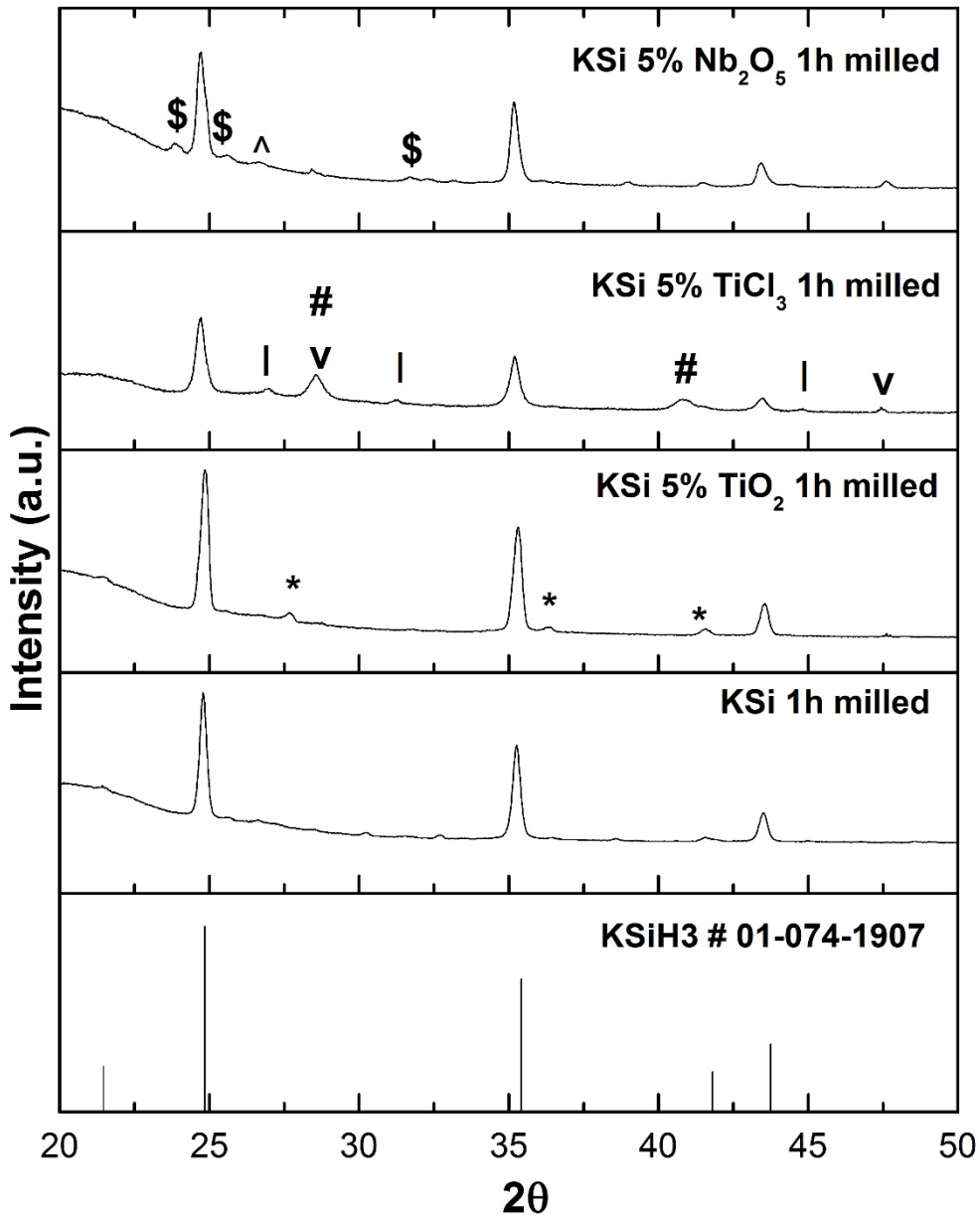

Fig. 2 XRD pattern of all hydrogenated KSi sample. Different phases are indexed by symbols (shown in brackets) as follows: TiO_2 # 01-084-1284 (*); KCl # 00-004-0587 (#); KH # 00-000-1263 (|); Nb_2O_5 # 00-019-0862 ($); NbO_2 # 01-071-4836 (^); Si # 01-080-0018 (v).

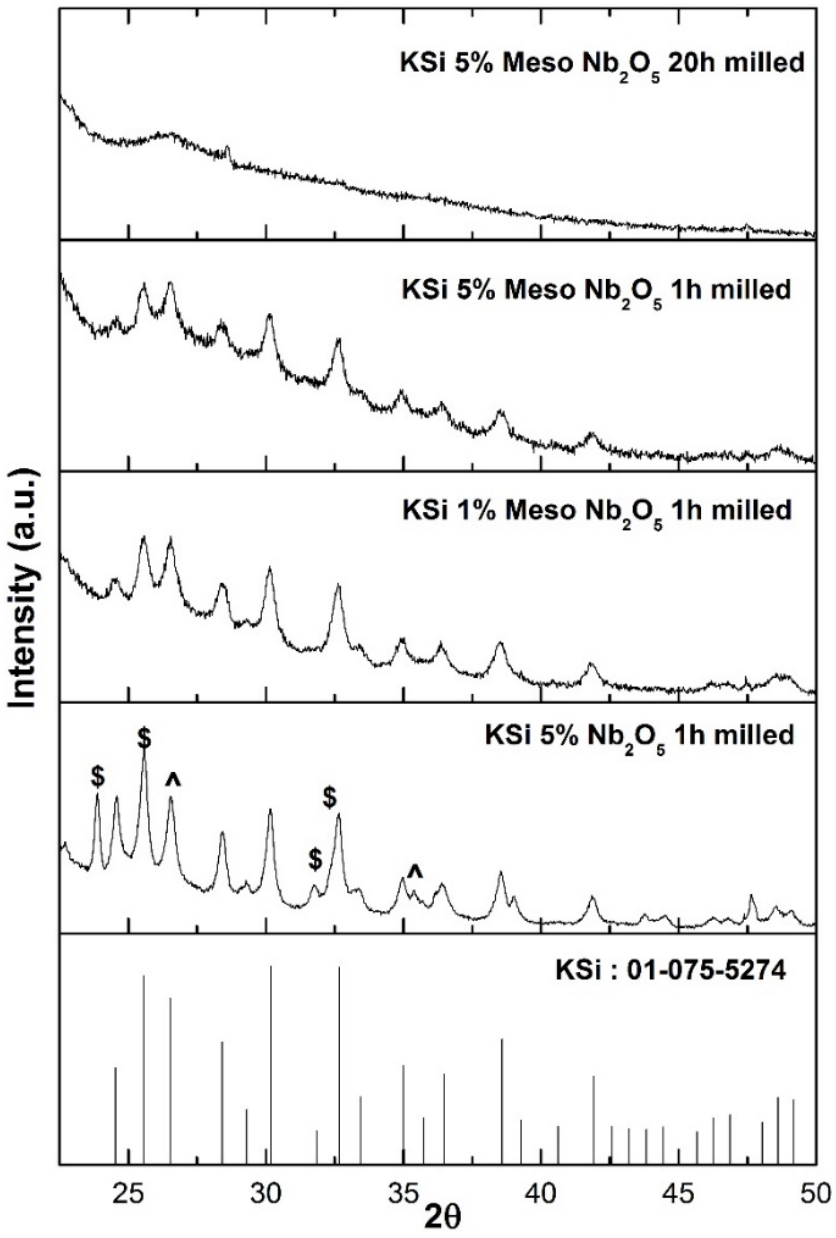

Fig. 3 XRD pattern of milled KSi samples with Nb_2O_5 by varying the the catalyst amount, milling time and particle size of catalyst. Different phases are indexed by symbols (shown in brackets) as follows: Nb_2O_5 # 00-019-0862 ($); NbO_2 # 01-071-4836 (^).

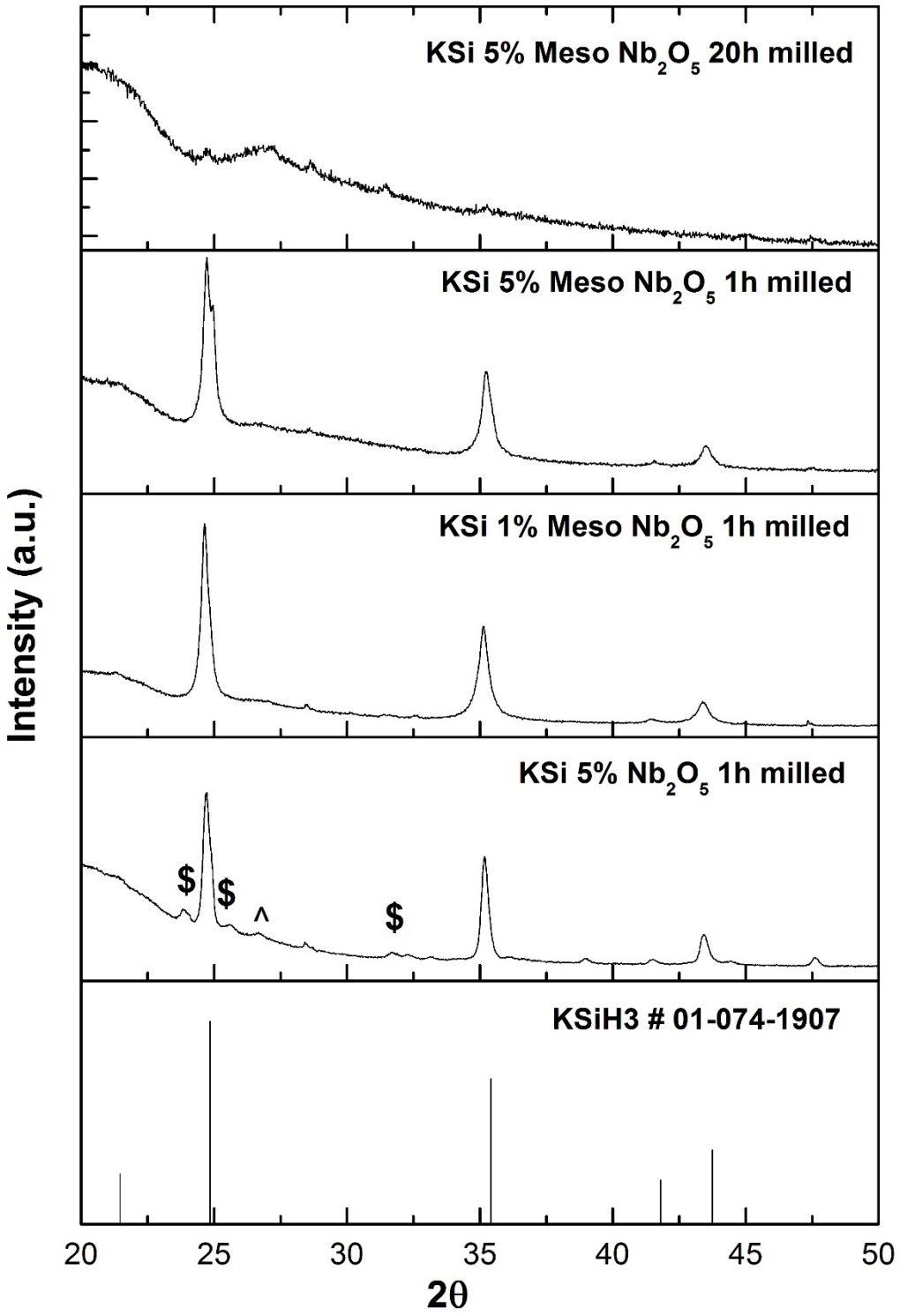

Fig. 4 XRD pattern of milled KSi samples with Nb_2O_5 by varying the catalyst amount, milling time and particle size of catalyst after hydrogenation. Different phases are indexed by symbols (shown in brackets) as follows: Nb_2O_5 # 00-019-0862 ($); NbO_2 # 01-071-4836 (^).

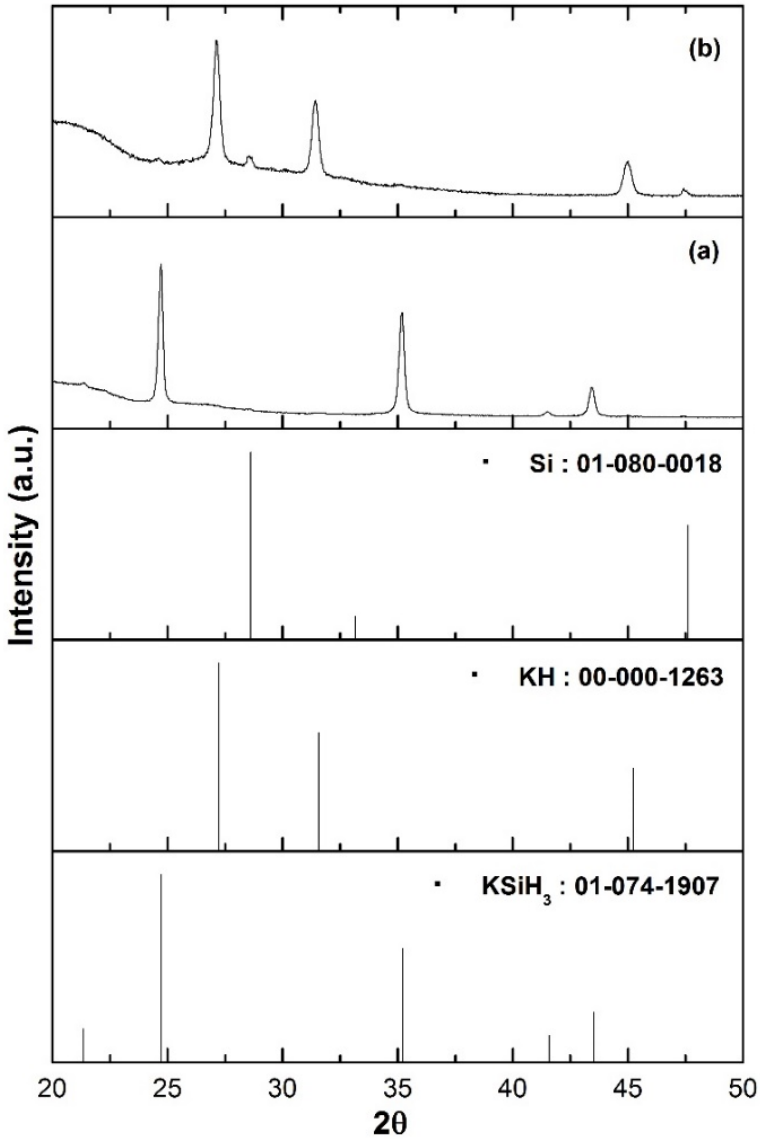

Fig. 5 XRD pattern of 1h milled KSi sample after hydrogenation following two different reaction environment (a) heated upto 100^{o}C with heating rate 10 ^{o}C/min after filling 5 MPa hydrogen (b) heating upto 100^{o}C with heating rate 10 ^{o}C/min under vacuum then introduce 5 MPa hydrogen instantly.

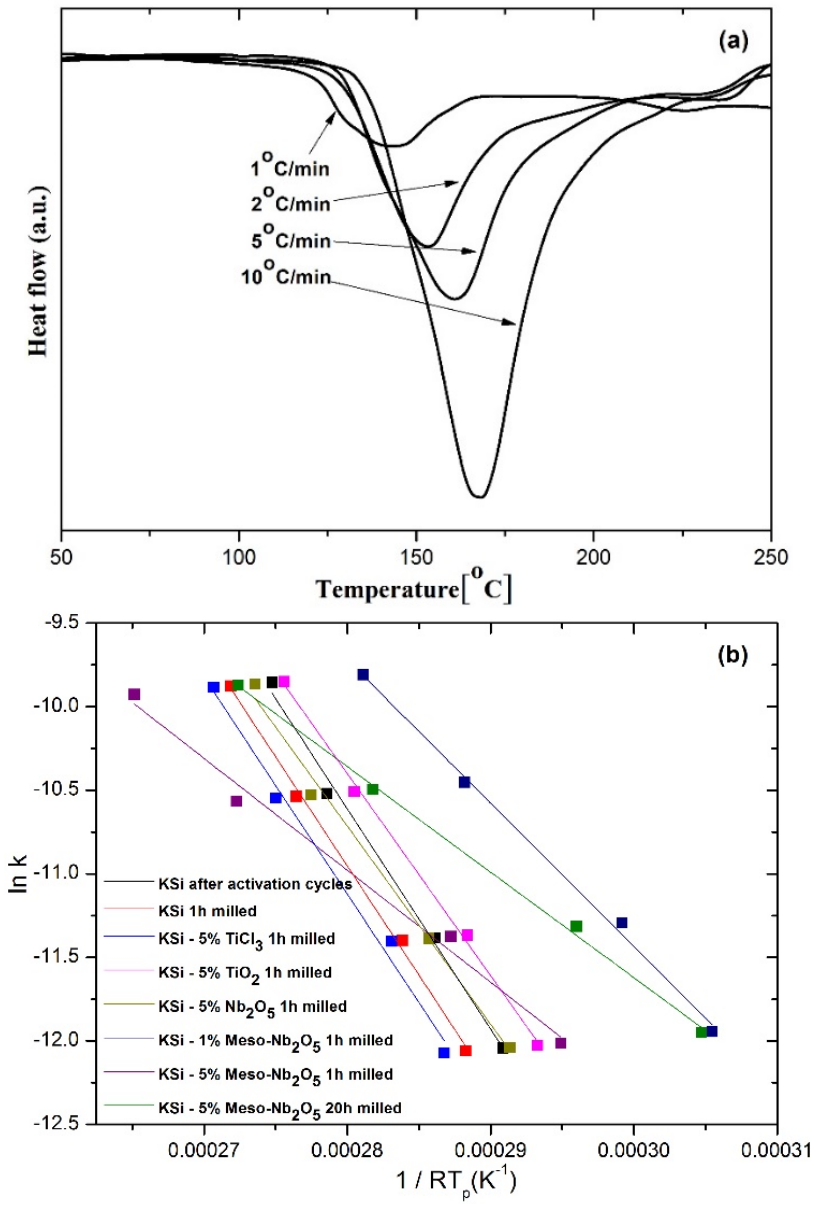

Fig. 6 (a) DSC curve of hydrogenated 1h milled KSi sample under 0.1 MPa Ar at 1, 2, 5, 10°C/min; (b) Kissinger plots using peak temperatures at different heating rates.

Table 1 Activation Energy corresponding to $KSiH_3 \rightarrow KSi$ conversion for all the samples

S. No.	Sample	Desorption Activation Energy E_{des} ($kJmol^{-1}$)
1	KSi after activation cycles	141.88 ± 6.67
2	1h milled KSi	130.58 ± 4.57
3	KSi – 5%$TiCl_3$ (1h milled)	129.861 ± 8.82
4	KSi – 5%TiO_2 (1h milled)	120.93 ± 3.72
5	KSi – 5% normal Nb_2O_5 (1h milled)	118.59 ± 7.32
6	KSi – 1% Mesoporous Nb_2O_5 (1h milled)	85.77 ± 3.34
7	KSi – 5% Mesoporous Nb_2O_5 (1h milled)	66.99 ± 4.624
8	KSi – 5% Mesoporous Nb_2O_5 (20h milled)	63.18 ± 1.91