Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Methane formation from the hydrogenation of Carbon dioxide on Ni (110) surface - A Density Functional Theoretical Study

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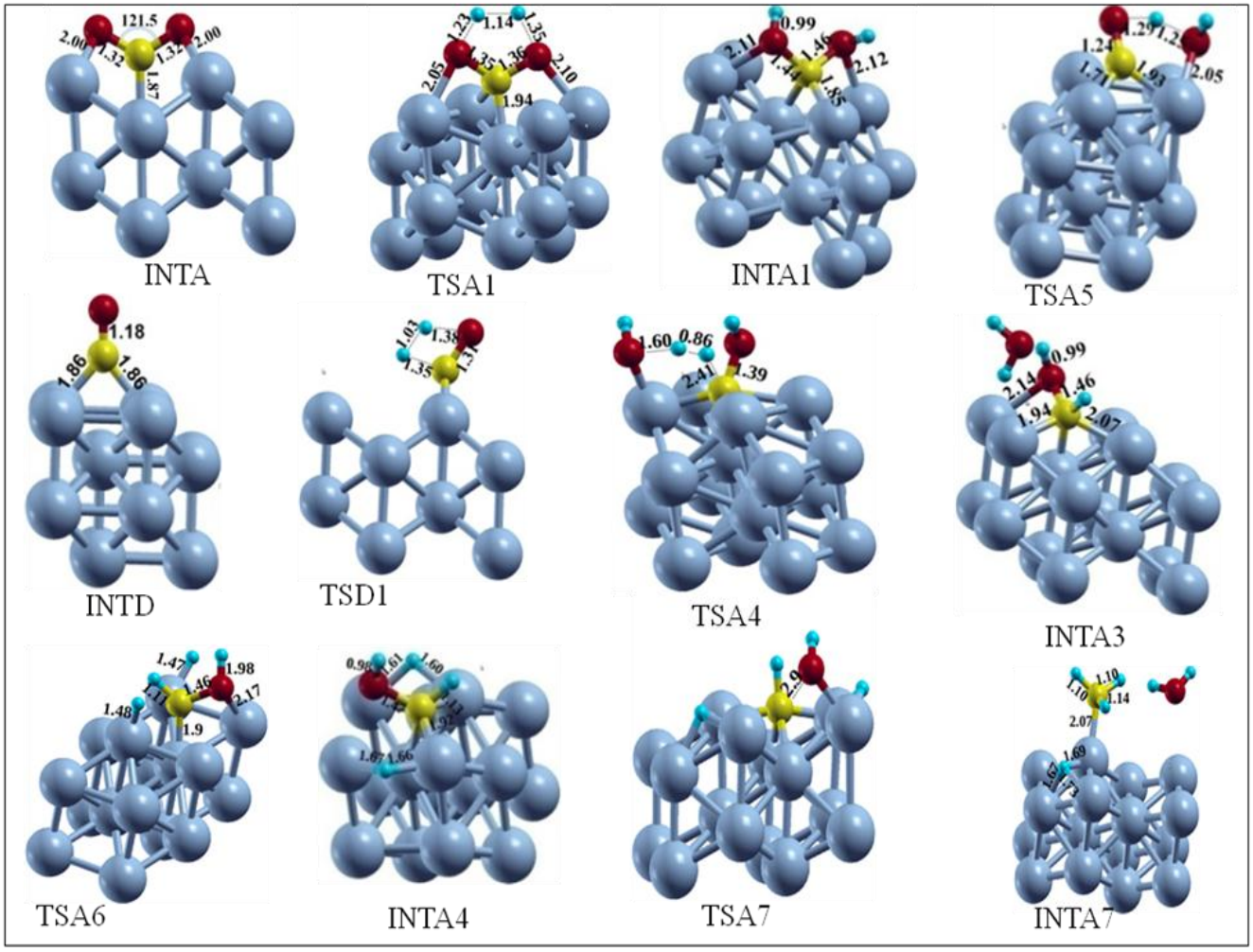
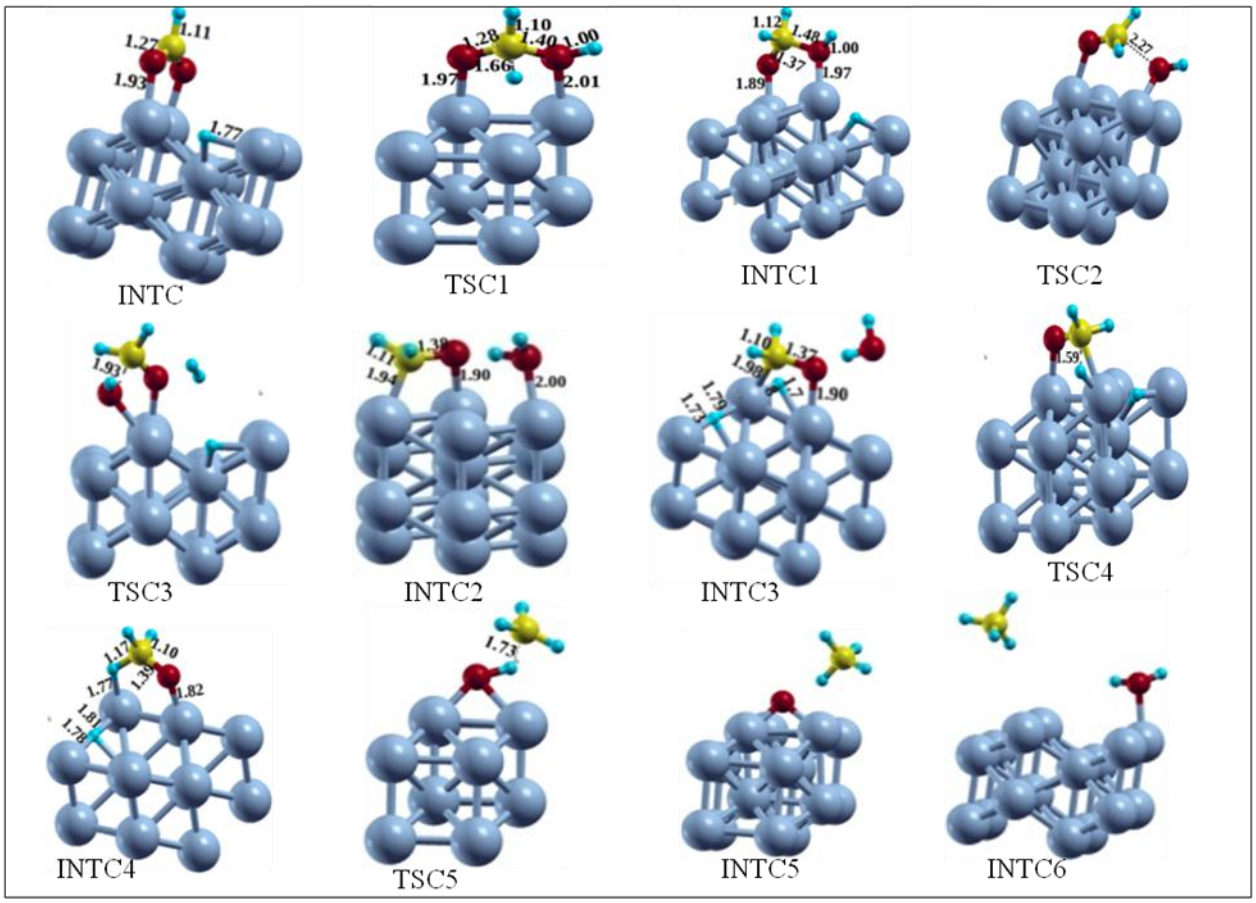


Fig S1. Possible intermediates and transition states of Fig. 2



FigS2. Possible intermediates and transition states of Fig. 4

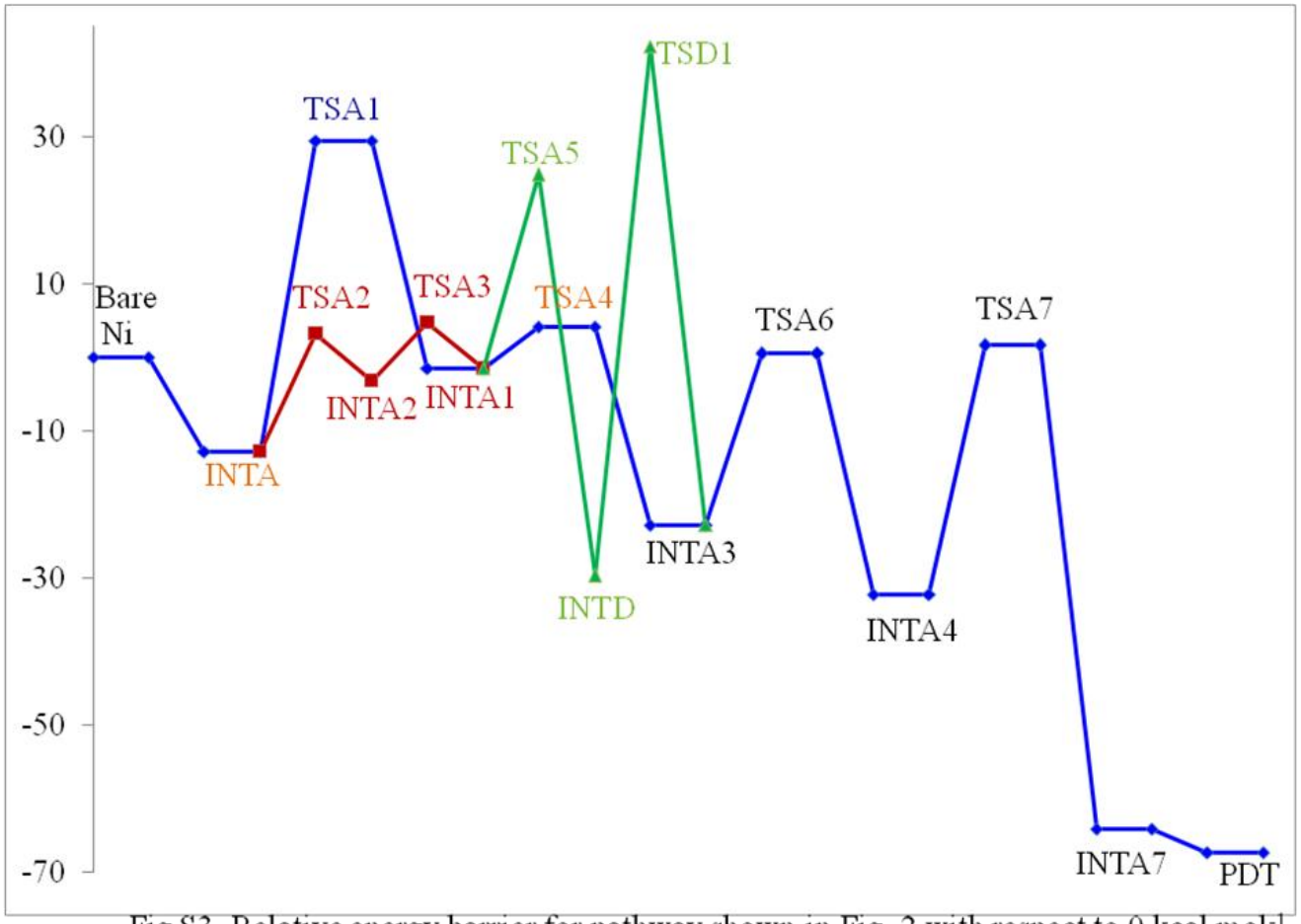


Fig S3. Relative energy barrier for pathway shown in Fig. 2 with respect to 0 kcal mol^{-1}

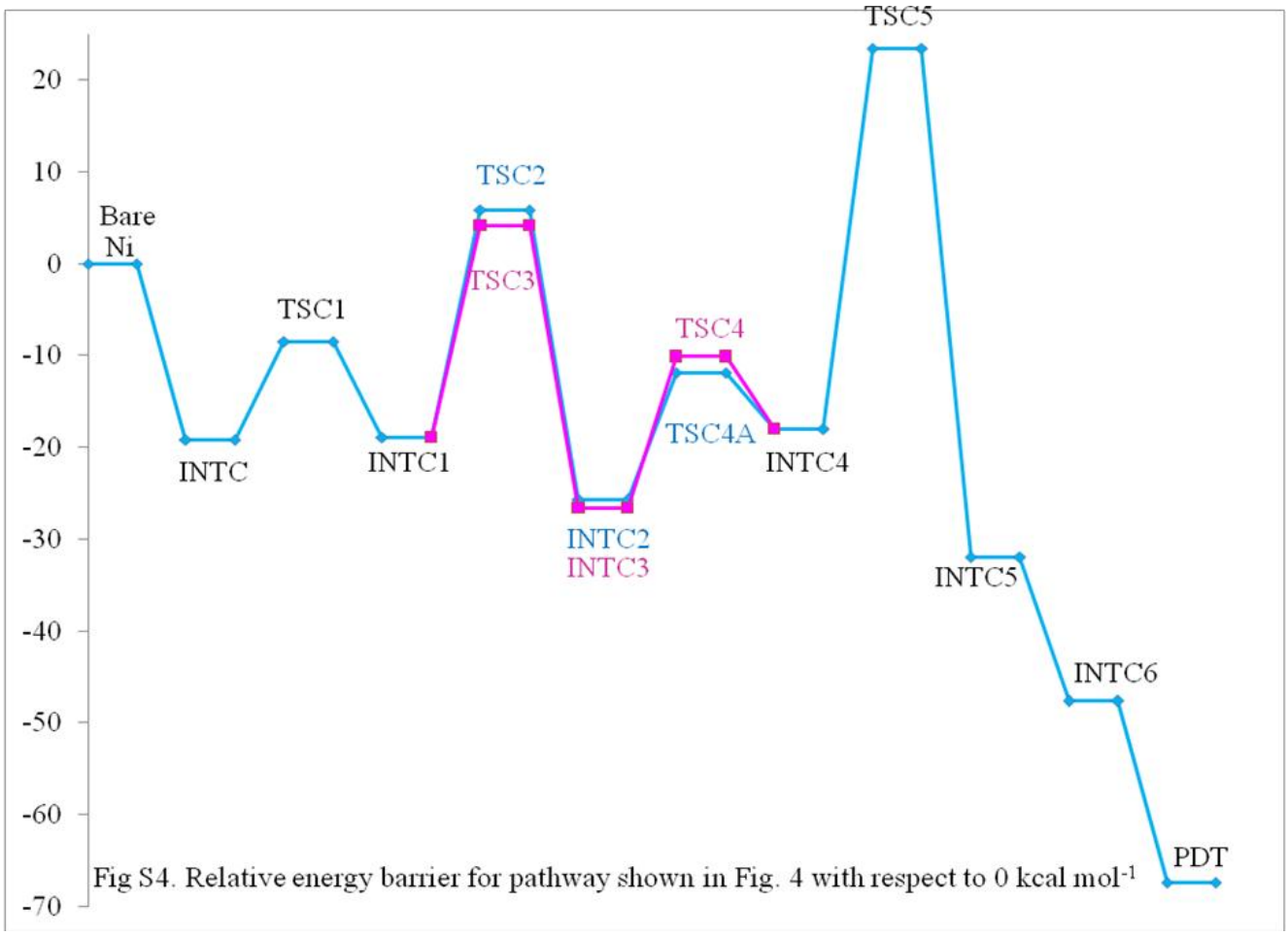


Fig S4. Relative energy barrier for pathway shown in Fig. 4 with respect to 0 kcal mol^{-1}

Species	Binding Energy(kcal mol^{-1})	Species	Binding Energy(kcal mol^{-1})
Nickel	0.00	INTB	-9.12
INTA	-12.87	INTC	-19.21
INTA1	-1.51	INTC1	-18.93
INTA3	-22.83	INTC2	-26.58
INTA4	-32.26	INTC3	-25.74
INTA7	-64.18	INTC4	-18.02
INTA2	-3.22	INTC5	-31.97
INTD	-29.73	INTC6	-47.68
PDT	-6 7.39		

TableS1: Binding Energies of different intermediates