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

Supporting Information for:

CO_2 activation and dissociation on the low miller index surfaces of pure and Ni-coated iron metal: a DFT study

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This supporting information contains information on all the other stable adsorption structures of CO_2, transition state structures, and structural parameters on the bare and Ni-deposited Fe (100), (110) and (111) surfaces. It contains six Figures and one Table.

Figure S1: Stable CO_2 adsorption modes on the Fe (100) surface. Colour code: Fe = pink, C = yellow and O = red.

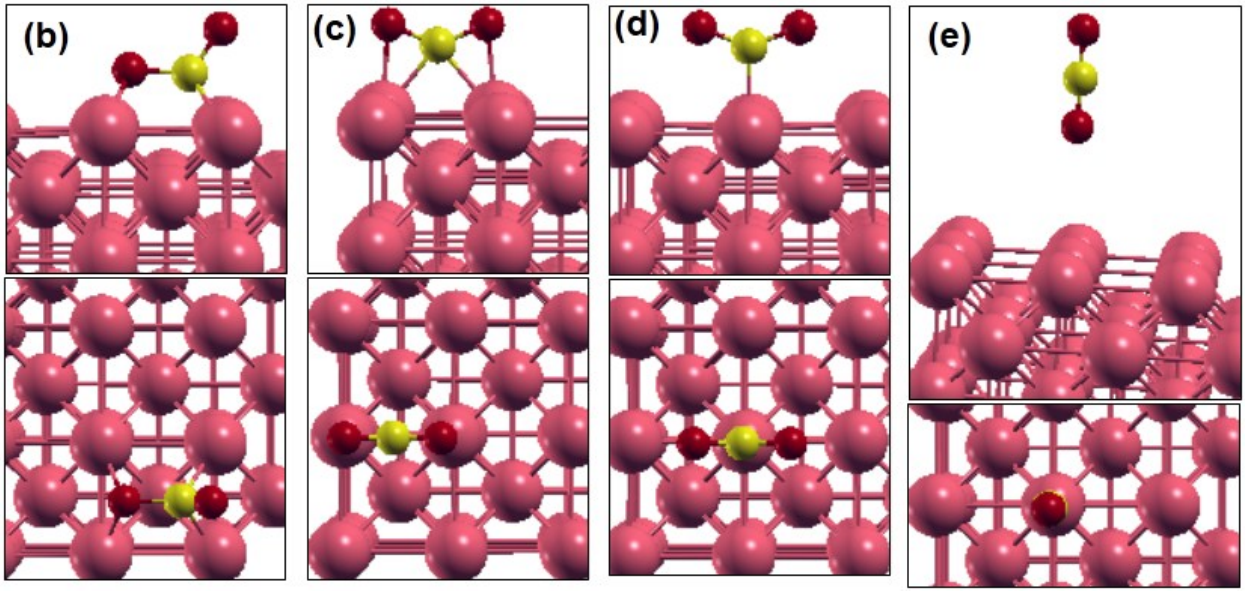

Figure S2: Stable CO_2 adsorption modes on the Fe (110) surface i.e. hollow-C_{2v} and bridge-C_{2v} configurations respectively.

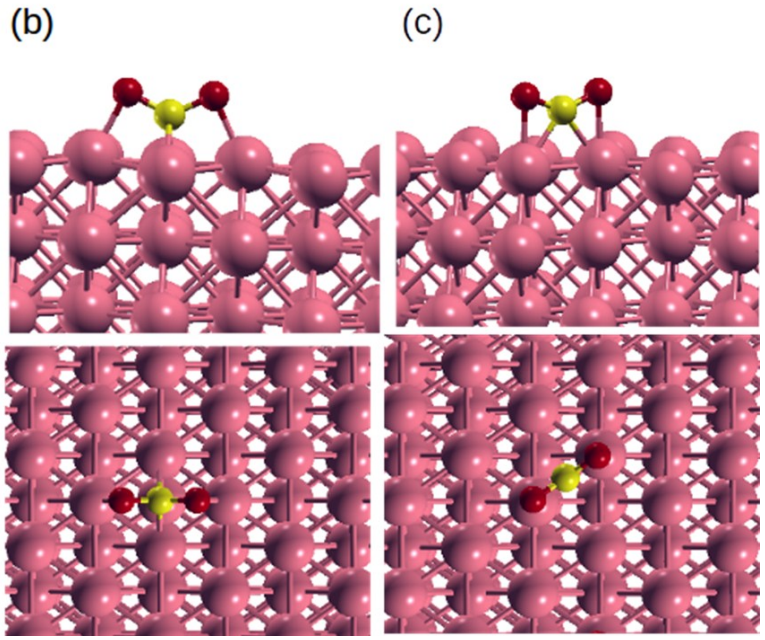

Figure S3: Stable CO_2 adsorption modes on the Fe (111) surface.

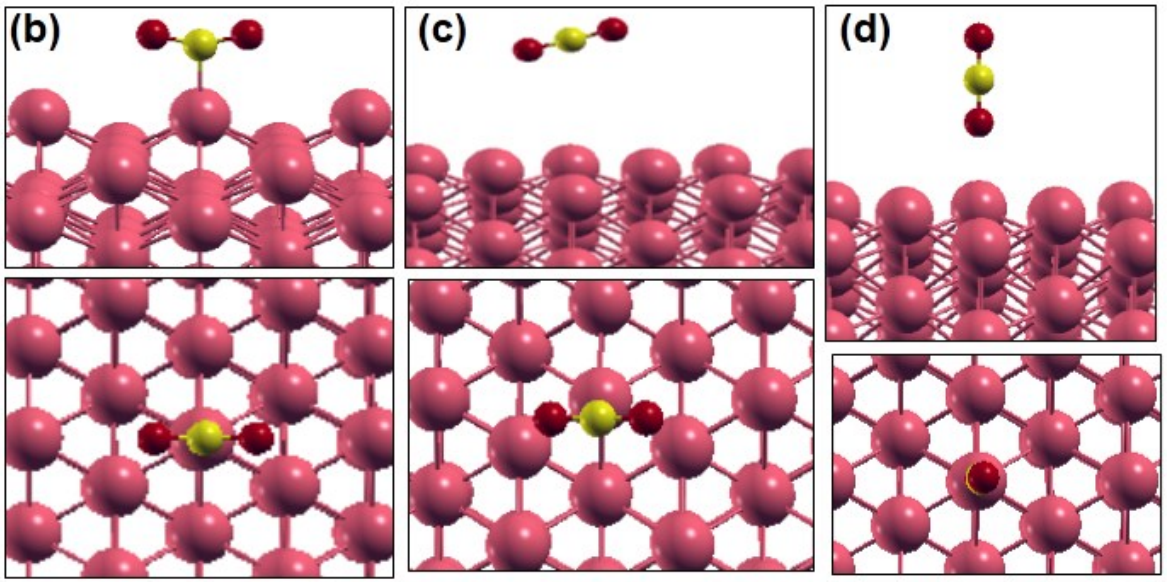

Figure S4: Geometries of stationary point structures along the reaction coordinate for CO_2 dissociation on bare Fe (100) (top) and on Ni-deposited Fe (100) (bottom).

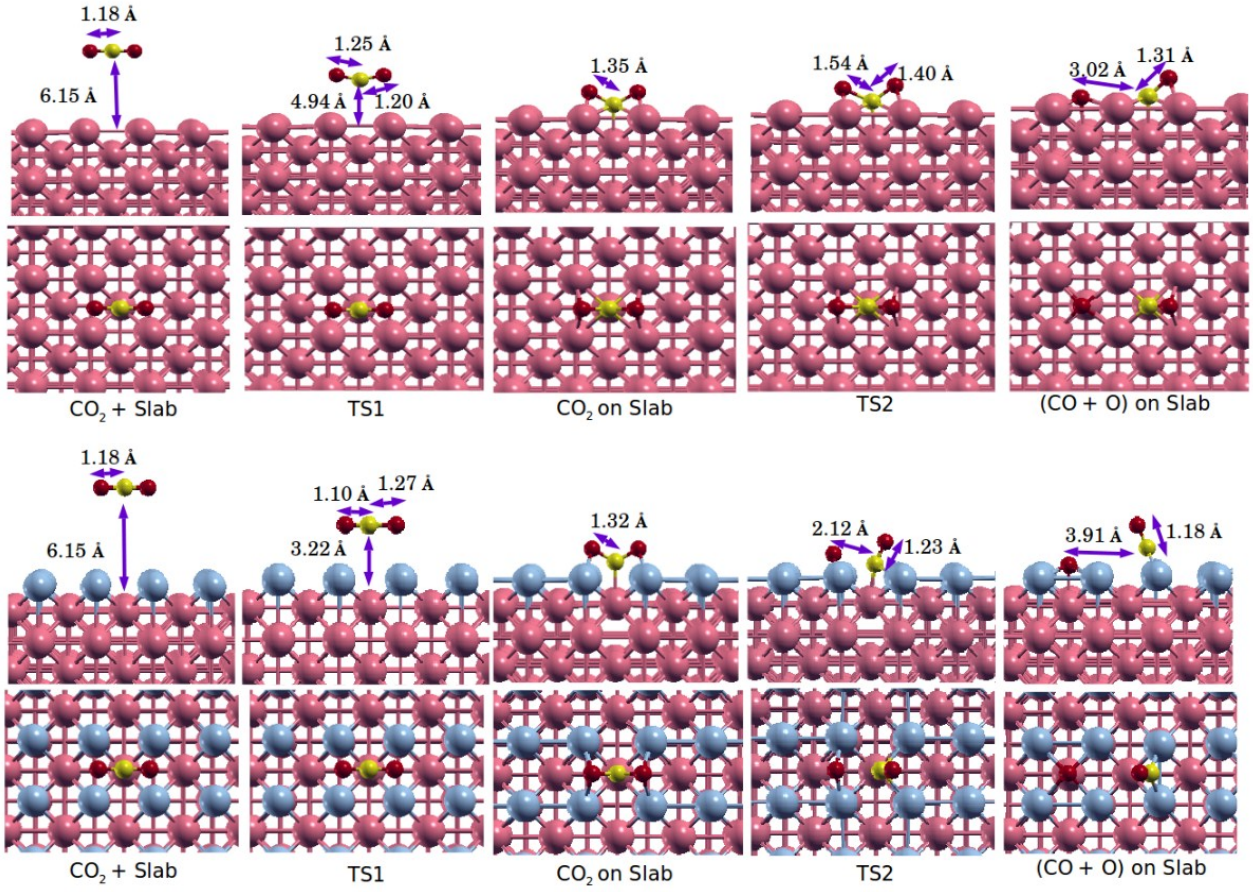

Figure S5: Geometries of stationary point structures along the reaction coordinate for CO_2 dissociation on bare Fe (110) (top) and on Ni-deposited Fe(110) (bottom).

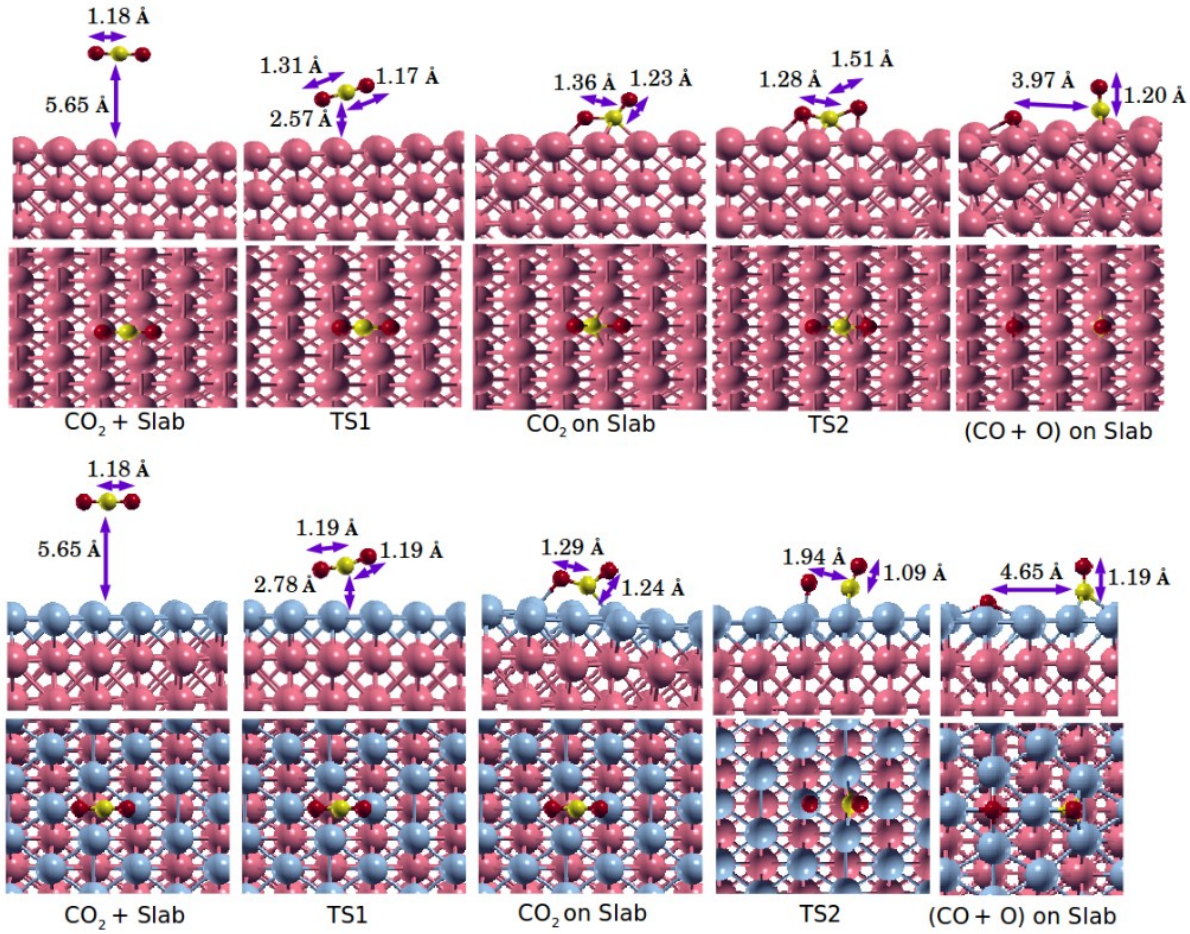

Figure S6: Geometries of stationary point structures along the reaction coordinate for CO_2 dissociation on bare Fe (111) and (top) and on Ni-deposited Fe(111) (bottom).

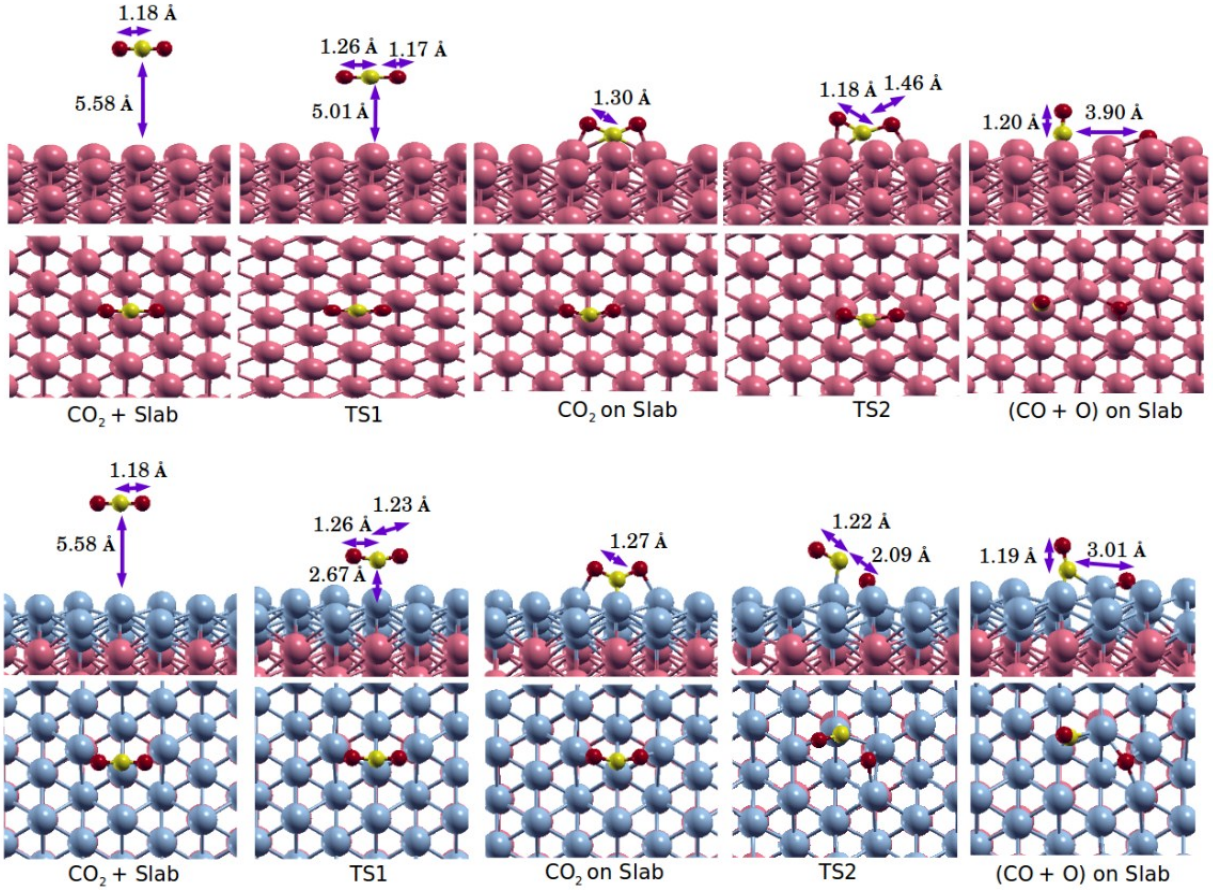

Table S1: Adsorption energy and structural parameters of CO_2 adsorbed on Fe (100), (110) and (111) surfaces.

Surface	Figure #	Structure	E_{ads} /kJmol^{-1}	C−O(1), C−O(2) /Å	O−C−O /°	Fe−C /Å	Fe−O(1), Fe−O(2) /Å	∑q /e
Fe(100)	S1-(b)	hollow-C_s	-53.7	1.24,1.39	121.86	2.11	2.04, 2.75	-0.06
	S1-(c)	bridge-C_{2v}	-62.7	1.26	134.91	2.08	2.11	-0.04
	S1-(d)	top-C_{2v}	15.4	1.25	138.71	1.95	2.66	-0.04
Fe(110)	S2-(b)	hollow-C_{2v}	-46.8	1.29	127.77	2.08	2.05	-0.06
	S2-(c)	bridge-C_{2v}	-45.6	1.25	137.23	2.09	2.13	-0.04
Fe(111)	S3-(b)	top-C_{2v}	27.1	1.22	151	2.10	2.68	-0.02
	S3-(c)	Top-linear-slanted	1.7	1.18,6.96	20.02	6.17	5.94, 6.59	0.00
	S3-(d)	Top-linear-vertical	-1.1	1.18,1.17	179.9	-	2.38	0.00