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

DFT Study of CO_2 Conversion on $InZr_3(110)$ Surface

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Table S1. The effect of the thinkness of the slab on the adsorption energy of CO species on $InZr_3(110)$ surface.

Thinkness of slab	4	5	6
Adsorption energy/eV	-2.92	-2.90	-2.88

Table S2. The effect of the number of thr k-points on the adsorption energy of CO species on $InZr_3(110)$ surface.

k-point	$3 \times 2 \times 2$	$4 \times 3 \times 2$	$5 \times 4 \times 3$
Adsorption energy/eV	-2.92	-2.90	-2.91