Supporting information

The Catalytic Reduction of Carbon Dioxide on the (001), (011), and (111) surfaces of TiC and ZrC: a Computational Study

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Table S1 Activation energy for CO_2 adsorption reported in this work compared to previously reported values[7].

			TiC			ZrC
	$^{a}E_r$	$^{b}E_r$	*%diff*	$^{a}E_r$	$^{b}E_r$	*%diff*
(001)	-0.90	-0.86	-0.05	-1.68	-1.62	-0.04
(011)	-3.45	-3.45	0.00	-4.19	-1.03	-3.07
(111)	-3.11	-3.05	-0.02	-3.17	-3.32	0.04

$^{a}\boldsymbol{E}_{\mathbf{r}}$ lowest energy CO_2 adsorption energy. $^{b}\boldsymbol{E}_{\mathbf{r}}$ previously reported CO_2 adsorption values using the geometry scan method[1]. ***%diff*** percentage between CO2 adsorption values determined using both methods.

References

(1) Quesne, M. G.; Roldan, A.; De Leeuw, N. H.; Catlow, C. R. A. Carbon Dioxide and Water Co-Adsorption on the Low-Index Surfaces of TiC, VC, ZrC and NbC: A DFT Study. *Phys. Chem. Chem. Phys.* **2019**, *21* (20). https://doi.org/10.1039/c9cp00924h.