Supplementary Information: Modeling the chemistry of Mn-doped MgO for bulk and (100) surfaces

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	CO_2 axis	B3LYP	B97-3
Mn_{surf}	x	-0.66	-0.74
	y	-0.74	-0.80
	z	0.00	-0.01
Mn_{sub}	x	-0.79	-0.86
	z	0.01	0.00
Mg [1]	x	-0.68	-
	z	0.12	-

Table 1 $E_{ads}(CO_2)$ on O_{5c} sites over Mn-MgO (100) surface. Also presented are previously calculated results for CO_2 adsorption on MgO using the B3LYP XC functional and similar basis sets. [1] All values are given in eV.

References

1 C. A. Downing, A. A. Sokol and C. R. A. Catlow, *Phys. Chem. Chem. Phys.*, 2014, **16**, 184–195.

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