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

Supporting information

Probing the nature of Lewis acid sites on oxide surfaces with $^{31}P(CH_3)_3$ NMR: A theoretical analysis

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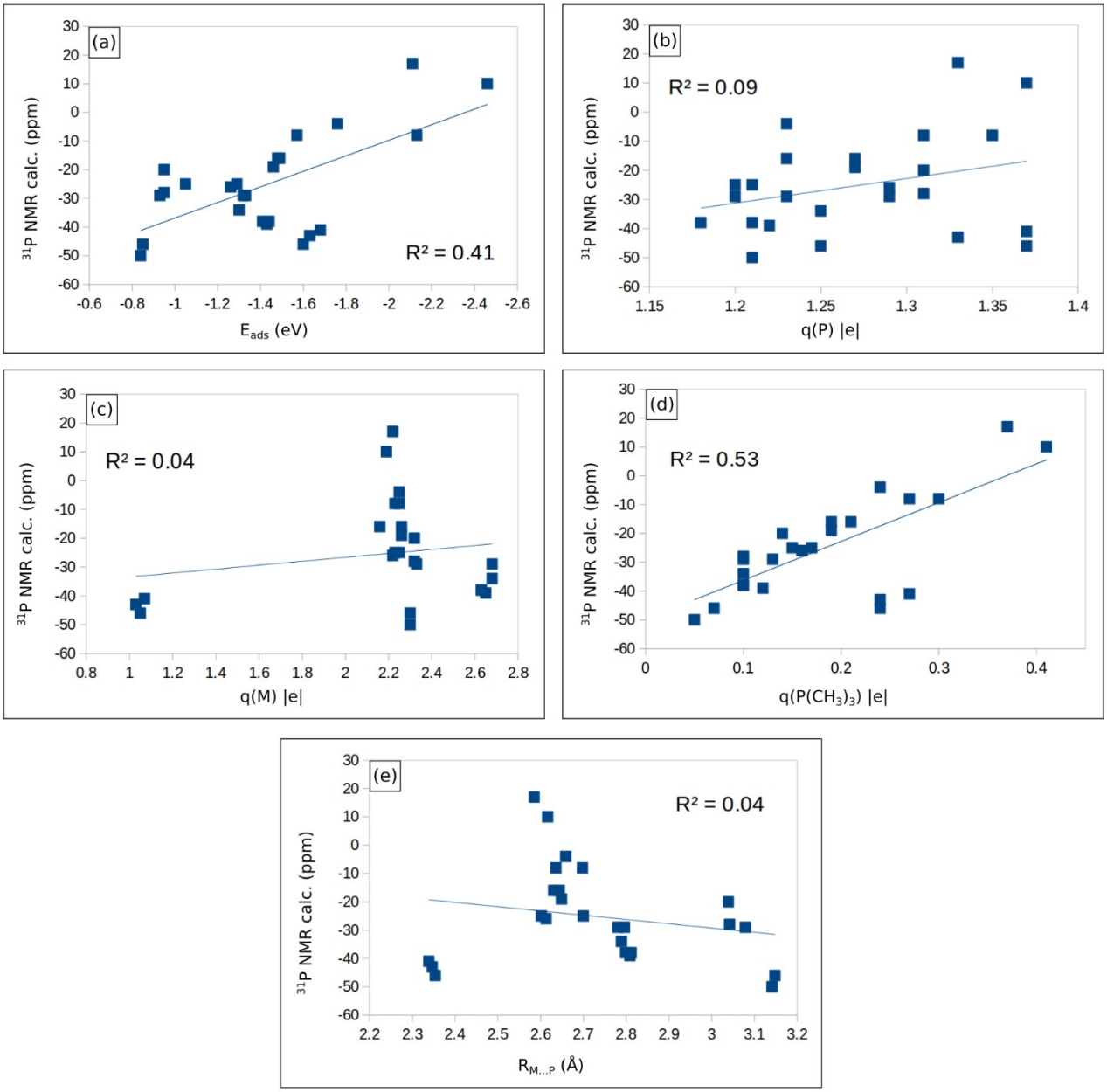

Figure S1 – Plot of computed ^{31}P chemical shift versus (a) adsorption energy, E_{ads}, (b) charge on P atom as obtained from Bader analysis, q_P, (c) charge on the surface cation where the TMP molecule is adsorbed, $q_{M...P}$, (d) net charge on the whole TMP molecule, $q_{P(CH3)3}$, (e) cation-P distance, $R_{M...P}$, see also Table 1. All data included.

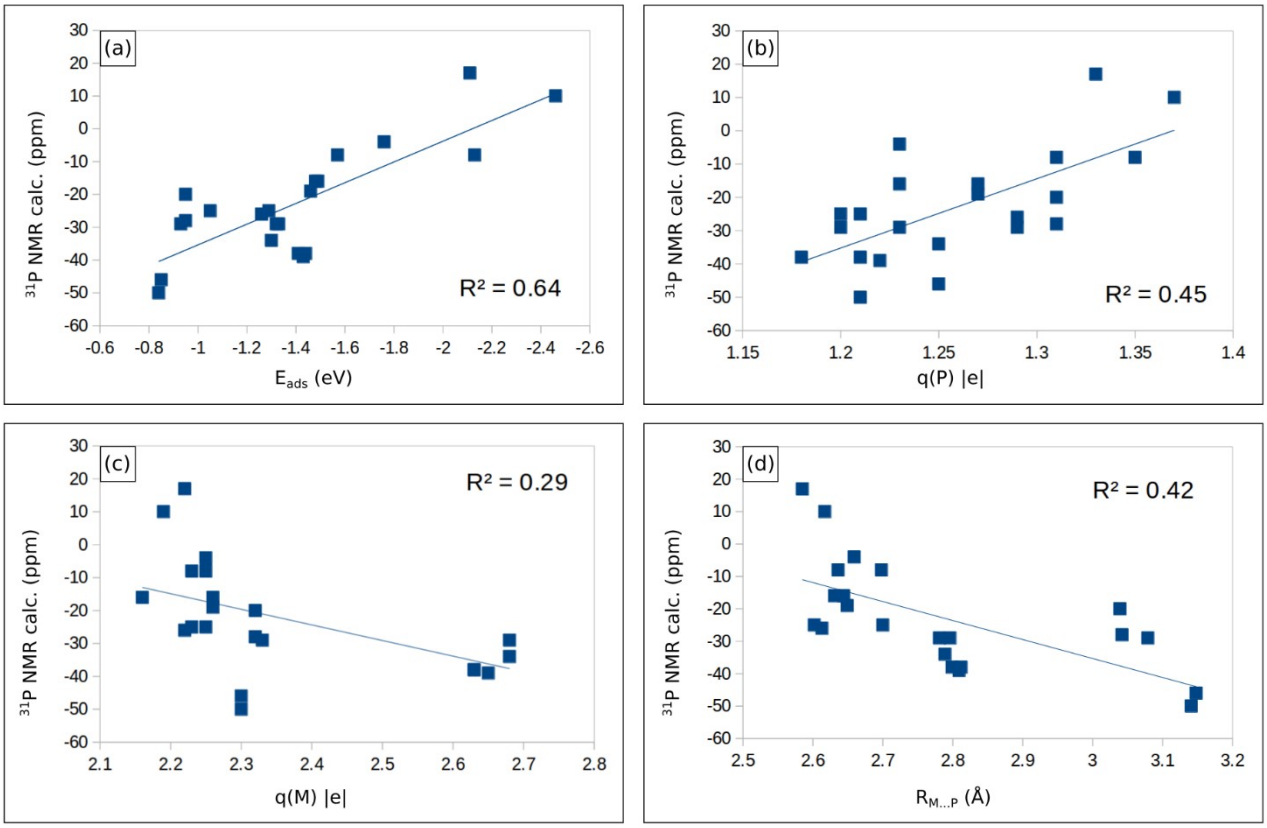

Figure S2 – Plot of computed ^{31}P chemical shift versus (a) adsorption energy, E_{ads}, (b) charge on P atom as obtained from Bader analysis, q_P, (c) charge on the surface cation where the TMP molecule is adsorbed, $q_{M...P}$, (d) net charge on the whole TMP molecule, $q_{P(CH3)3}$, (e) cation-P distance, $R_{M...P}$, see also Table 1. Data referred to ZnO not included.

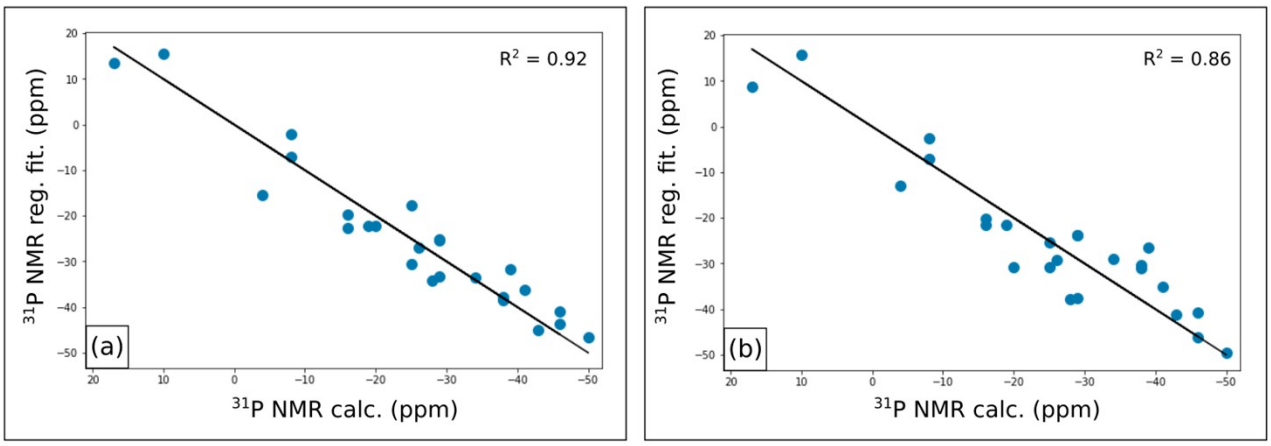

Figure S3 - Correlation between ^{31}P NMR calculated and regression fitted by considering (a) adsorption energy (E_{ads}) and Bader charges ($q(P(CH_3)_3)$ and q(M)) and (b) work functions (Φ) and Bader charges ($q(P(CH_3)_3)$ and q(M)), see Table 1.

Table S1. The coefficients of regression models for normalized set of data shown in Figure S3.

	a	b	c
Fig S3a	0.62	0.75	1.61
Fig S3b	0.08	0.60	0.95