Electronic Supplementary Material (ESI) for Catalysis Science & Technology

Kinetic Monte Carlo Simulations for Model Catalysis of Heterogeneously Catalyzed Oxidation Reactions

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Supporting Information

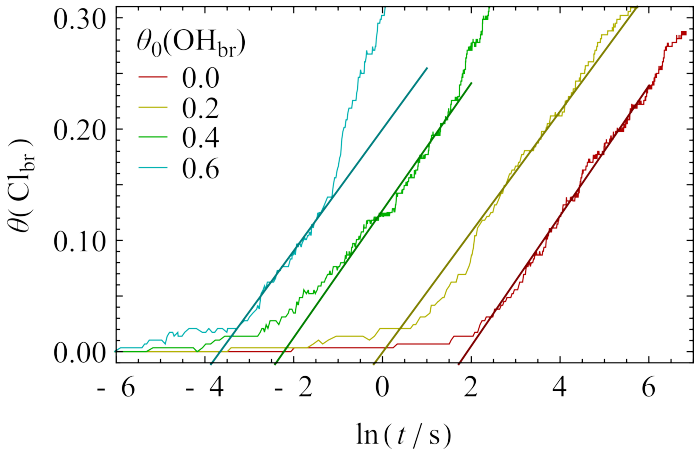

Figure S1: about the determination of τ_0 Values for the chlorination of $RuO_2(110)$ (Section 3.3.3). Chlorination curves were simulated with kMC and $\theta(Cl_{br})$ was plotted as a function of $\ln(t/s)$. The curves revealed quasi-linear segments which were fitted with a linear function $\theta(Cl_{br}) = a \ln(t/s) + b$. The induction time τ_0 is the intercept of the straight with the abscissa and can be expressed by $\tau_0 = e^{-\frac{b}{a}}$.