**Electronic Supplementary Information**

**Supp. S1.** Calculated structural isomers for Ti$_2$O$_4^+$ given in eV. The gray isosurfaces indicate localized spin density.

**Supp. S2.** (a) Snapshots from MD simulations of the reaction TiO$_2^+$ with CO performed at constant energy (E = 0.1 eV). Branching ratios presented in normalized ion intensities for reaction of TiO$_2^+$ with (b) CO, (c) C$_3$H$_6$, (d) C$_2$H$_2$ and (e) C$_2$H$_4$. (f) Snapshots from MD simulations performed at constant temperature (T = 1500 K) of the reaction Ti$_2$O$_4^+$ with C$_2$H$_2$. 
Supp. S3. (a) A calculated energy profile given in eV for reaction of Ti$_2$O$_4^+$ with C$_3$H$_6$ forming propanal differing with Figure 3 through an isomerization. (b) An additional calculated energy profile given in eV for reaction of Ti$_2$O$_4^+$ with C$_3$H$_6$ forming an epoxide. This mechanism is endothermic.