SUPPORTING INFORMATION

The Interaction of H₂O₂ with TiAlPO-5 Molecular Sieves. Probing the Catalytic Potential of Framework Substituted Ti Ions.

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S1 UV-Vis spectra of calcined TiAlPO-5 reacted with aqueous H₂O₂.

Figure S1. DR UV-Vis spectra of a) Calcined TiAlPO-5, b) in contact with aqueous H₂O₂ and c) after room temperature outgassing. Spectra were arbitrarily normalized for easier comparison.
S2. Experimental ENDOR Spectra

Figure S2. Experimental Mims ENDOR spectra of O\textsubscript{2} on TiAlPO-5 obtained by reaction of the calcined sample with A) hydrated H\textsubscript{2}O\textsubscript{2} and B) anhydrous H\textsubscript{2}O\textsubscript{2} (from UHP). The spectra are taken at three different magnetic field settings corresponding to a) $g_{zz}$ component ($B_0 = 344.4$ mT), b) $g_{yy}$ component ($B_0 = 346.6$ mT) and c) $g_{xx}$ component ($B_0 = 348.3$ mT).
S3. Computer simulations of $^{31}$P ENDOR spectra of TiAlPO-5 obtained by reaction with anhydrous H$_2$O$_2$ (from UHP)

Figure S3. Experimental (black line) and simulated (grey line) $^{31}$P Mims ENDOR spectra of O$_2^-$ on TiAlPO-5 obtained by reaction of the calcined sample with anhydrous H$_2$O$_2$ (from UHP) measured at three different magnetic field settings corresponding to a) $g_{zz}$ component ($B_0 = 344.4$ mT), b) $g_{yy}$ component ($B_0 = 346.6$ mT) and c) $g_{xx}$ component ($B_0 = 347.7$ mT). The asterisk indicates the $^{31}$P signal belonging to the remote phosphorous nuclei, which are not taken into account in the simulation. The simulated parameters are listed in Table 1 in the main text.