The ethylene epoxidation cycle in a $H_2O_2/H_2O$-loaded Ti zeolite has been simulated by a Car−Parrinello approach. Results indicate a process where the zeolitic framework is the active oxygen mediator. The dissociative chemisorption of $H_2O_2$ leads, via a transient Ti−hydroperoxo species, to $H_2O$ and a Ti−peroxo zeolite intermediate. Transfer of active oxygen to ethylene follows, giving the epoxide and recovering the catalyst. A thorough theoretical characterization indicates that the active oxidizing species is an asymmetric $\eta^2$-Ti−peroxo, absorbing in the visible range. The lability of the intermediate is found related to $\eta^2 \leftrightarrow \eta^1$ interconversions of the Ti−peroxo structure. The interconversions, triggered by water molecules, could account for the experimentally found reduced catalytic activity in aged TS-1 catalysts. The results provide a microscopic picture of the reactivity and dehydration/aging processes of the catalyst fully consistent with experiments and highlight the fundamental role of the Lewis acid character of Ti in the formation, reactivity, and degradation of the active oxidizing species.