Using ab initio modelling, we demonstrate that H atoms can break strained Si-O bonds in continuous amorphous silicon dioxide (a-SiO$_2$) networks resulting in a defect which we call the hydroxyl E’ centre. Unlike crystalline silicon dioxide, where neutral H atoms occupy interstitial positions and exhibit negative U behaviour, the neutral hydroxyl E’ centre in a-SiO$_2$ is thermodynamically stable in a number of configurations over a range of Fermi levels.

More than 100 models of a-SiO$_2$, each containing 216 atoms, were generated in order to model the distribution of the defects’ properties using a classical potentials and a melt-and-quench technique and further relaxed using DFT. The non-local functional PBE0_TC_LRC was used to accurately model the defect levels in the CP2K code. The hydroxyl E’ centres are produced when H atom reacts with strained Si-O bonds which requires overcoming a barrier of 0.5 to 1.3 eV, dependent on the local environment. Due to disorder, the defect levels are spread over a 2 eV range. We also find that the hydroxyl E’ centre can trap a hole or an extra electron as well as take part in further reactions with H atoms and H$_2$ molecules.