Liquid Helium becomes superfluid and frictionless at very low temperature. We are interested in the superfluid properties of helium and hydrogen clusters doped with molecular impurities. Molecular hydrogen has been suggested as a potential candidate but this substance crystallizes before reaching a temperature low enough for superfluidity to appear. We will show theoretical and experimental results that demonstrate the possibility of obtaining a molecular superfluid response at the nanoscale via the formation of doped hydrogen clusters. The theoretical results are based on the path integral description of quantum statistical mechanics. We will discuss the advantages of this approach for the quantum simulation of complex molecular systems. Properties such as density distributions and spectral features can be extracted from the simulations. We will present new results for the case of asymmetric top molecules embedded in superfluid para-hydrogen clusters.