Interstellar grains are thought to play an important role in the formation of complex molecules in the interstellar medium [1]. However, the low temperature and scarcity of reactants present in their ice mantle strongly limit the formation of complex molecules in their bulk. Whether or not long time scale can counterbalance this diffusion-limited solid-state reactivity at low-temperature strongly depends on the diffusion coefficients of the reactants.

I will present our combined theoretical and experimental study on the diffusion of a series of small molecules in amorphous ice. I will first detail the classical Molecular Dynamics simulations undertaken to model the amorphous ice and to calculate the diffusion coefficient of H$_2$O, CO$_2$, NH$_3$, CO and H$_2$CO in the bulk of this ice. I will then present our experimental setup and the protocols used to study the diffusion of CO$_2$ and its thermal dependance in the same type of ices. I will finally compare the diffusion coefficients and their temperature-dependance derived from both present and previous experiments to our theoretical calculations, and will comment on a plausible water-mediated diffusion mechanism.