ASYMMETRIC TOP ROTORS IN SUPERFLUID PARA-HYDROGEN NANO-CLUSTERS

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We present the first simulation study of bosonic clusters doped with an asymmetric top molecule. A variation of the path-integral Monte Carlo method is developed to study a para-water (pH$_2$O) impurity in para-hydrogen (pH$_2$) clusters. The growth pattern of the doped clusters is similar in nature to that of the pure clusters. The pH$_2$O molecule appears to rotate freely in the cluster due to its large rotational constants and the lack of adiabatic following. The presence of pH$_2$O substantially quenches the superfluid response of pH$_2$ with respect to the space fixed frame. We also study the behaviour of a sulphur dioxide ($^{32}$S$^{16}$O$_2$) dopant in the pH$_2$ clusters. For such a heavy rotor, the adiabatic following of the pH$_2$ molecules is established and the superfluid renormalization of the rotational constants is observed. The rotational structure of the SO$_2$-p(H$_2$)$_N$ clusters’ ro-vibrational spectra is predicted. The connection between the superfluid response respect to the external boundary rotation and the dopant rotation is discussed.