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_2O) 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_2O molecule appears to rotate freely in the cluster due to its large rotational constants and the lack of adiabatic following. The presence of pH_2O 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 SO₂- $p(H_2)_N$ clusters' ro-vibrational spectra is predicted. The connection between the superfluid response respect to the external boundary rotation and the dopant rotation is discussed.