Molecular assemblies are often described using classical concepts and simulated using Newtonian dynamics or Classical Monte Carlo methods. At low temperatures, this classical description fails to capture the nature of the dynamics of molecules, and a quantum description is required in order to explain and predict the outcome of experiments. In this context, the Feynman path integral formulation of quantum mechanics is a very powerful tool that is amenable to large-scale simulations [1]. We will show how path integral simulations can be used to predict the properties of molecular rotors trapped in superfluid helium and hydrogen clusters [2]. We will show that microscopic Andronikashvili experiments can be viewed as a measurement of superfluidity in a quantum mechanical frame of reference. We will also show that path integral ground state simulations can be used to predict the Raman spectra of parahydrogen clusters [3] and solids. We will present ongoing work on the simulation of molecular rotors confined in endohedral fullerene materials such as H2O@C60 and HF@C60 [4]. The questions we will address include symmetry breaking, spin conversion, the nature of dipole correlations and dielectric response, and entanglement measures [5-7] in assemblies such as peapods (Fig. 1) and two-dimensional solids.

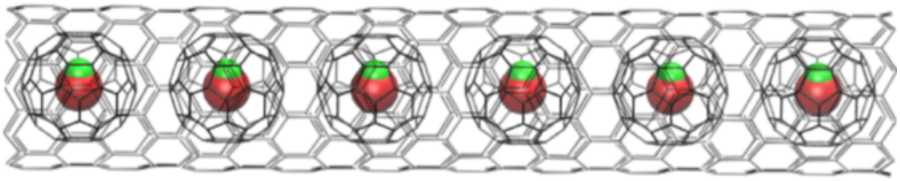

Fig. 1 Cartoon representation of an endofullerene peapod.

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