Quantization of vibrations in H-bonded crystals

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In this talk I will present a general methodology to include the effect of the quantization of vibrations on the structural and dynamical properties of crystals and molecules. The method is based on mapping a suitable subspace of the vibrational manifold and solving the Schroedinger equation in it, in a series of increasingly accurate approximations. I will present results for a model monoatomic chain and a hydrogen-bonded diatomic chain, and analyze them in detail. I will then show results for a more realistic case of a hydrogen-bonded linear F-H chain described at a first-principles level.

The focus is placed specifically on quantum nuclear effects on lattice constants and interatomic parameters.[1] A truly realistic application that solves a long standing question will be presented by K. Refson.

[1] I. Scivetti, N. Gidopoulos, and J. Kohanoff, Phys. Rev. B 78, 224108 (2008)