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The role of quantum nuclear effects in hydrogen bonded crystals and their calculated NMR shielding constants[1] KJARTAN THOR WIKFELDT, London Centre for Nanotechnology, University College London, CHRIS PICKARD, Department of Physics and Astronomy, University College London, ANGELOS MICHAELIDES, London Centre for Nanotechnology, University College London — Because of its ubiquity in nature the hydrogen atom plays a very important role in computational materials science. As the lightest element, hydrogen nuclei are also the most strongly affected by quantum nuclear effects (QNEs). The path integral (PI) formalism provides a rigorous approach to obtain equilibrium quantum static properties, but PI simulations in conjunction with electronic structure calculations are rarely used due to high computational requirements. This contribution will discuss ab initio PI simulations aimed at elucidating the role of QNEs in hydrogen bonded crystals and how these impact upon experimental observables such as nuclear magnetic resonance (NMR) shielding constants and chemical shifts. We find that ab initio PI simulations improve the agreement with experimental chemical shifts compared to simulations with classical nuclei and that the influence of QNEs is very sensitive to the strength of the hydrogen bonds in the crystal.

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