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The isotope effect in the ferroelectric phase transition of KDP using *ab-initio* path intergal simulations VARADHARAJAN SRINIVASAN[1], ROBERTO CAR, Princeton University, Princeton, NJ 08544, US, DANIEL SEBASTIANI, Max Planck Institute for Polymer Research, Ackermannweg 10 / 55128 Mainz, Germany — We perform *ab-initio* path integral simulations on protonated and deuterated KDP at different temperatures and lattice constants in order to probe the origin of the isotope effect of the ferroelectric phase transition in this material. By taking into account the quantum nature of the proton/deuteron our simulations are capable of distinguishing the direct effects of a pure mass change versus the indirect structural effect in the hydrogen bonding geometry upon deuteration. In reality, the direct and indirect effects amplify each other in a self-consistent manner, leading to the huge isotope effect on the transition temperature. With our calculation we can selectively investigate the manisfestation of the two phenomena. We characterize the ferro and paraelectric phases with the help of a recent modification of the path integral implementation in the CPMD package which enables us to compute momentum distributions of the proton/deuteron both above and below the transition temperature in order to characterize the extent of proton/deuteron delocalization in both phases.

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