

# Isotope effects on water responsive materials: HYF and Water vs Heavy Water

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Water responsive (WR) materials can undergo reversible changes in their conformation in response to relative humidity (RH) changes. They have recently gained attention due to their opportunities to be used as an energy source. Evaporation-driven engines, for example, can be powered by WR materials to directly harvest energy from the natural evaporation of water and convert it into mechanical work and electricity. However, little is known about the mechanisms involved in these WR materials or the role of water in these systems. In particular, the effects of deuterium oxide ( $D_2O$ ) on the mechanical properties of WR materials and the interactions between water and biomolecules is still an open question. In this study, we compared the responsiveness of histidine-tyrosine-phenylalanine (HYF) peptide crystals to  $H_2O$  and  $D_2O$  and the role of nanoconfined water in the water-peptide interactions. We investigated the changes in the mechanical properties of HYF due to isotope substitution ( $H_2O$  and  $D_2O$ ). We performed experiments using powder x-ray diffraction (PXRD), atomic force microscopy (AFM), and Fourier-transform infrared spectroscopy (FTIR) in a humidity-controlled environment with both,  $H_2O$  and  $D_2O$  vapor to study its RH responsiveness. We also complement our experiments by performing classical and path-integral molecular dynamics simulations.