Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Phosphate vibrations as reporters of DNA hydration STEVEN CORCELLI, Univ of Notre Dame — The asymmetric phosphate stretch vibrational frequency is extraordinarily sensitive to its local solvent environment. Using density functional theory calculations on the model compound dimethyl phosphate, the asymmetric phosphate stretch vibrational frequency was found to shift linearly with the magnitude of an electric field along the symmetry axis of the PO_2 moiety (i.e. the asymmetric phosphate stretch is an excellent linear vibrational Stark effect probe). With this linear relationship established, asymmetric phosphate stretch vibrational frequencies were computed during the course of a molecular dynamics simulation of fully hydrated DNA. Moreover, contributions to shifts in the frequencies from subpopulations of water molecules (e.g. backbone, minor groove, major groove, etc.) were calculated to reveal how phosphate vibrations report the onset of DNA hydration in experiments that vary the relative humidity of non-condensing (dry) DNA samples.

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Date submitted: 14 Sep 2016 Electronic form version 1.4