Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nuclear Quantum Effects in the Dynamics of Biologically Relevant Systems from First Principles MARIANA ROSSI, University of Oxford, UK, WEI FANG, ANGELOS MICHAELIDES, University College London, UK — Understanding the structure and dynamics of biomolecules is crucial for unveiling the physics behind biology-related processes. These molecules are very flexible and stabilized by a delicate balance of weak (quantum) interactions, thus requiring the inclusion of anharmonic entropic contributions and an accurate description of the electronic and nuclear structure from quantum mechanics. We here join state of the art density-functional theory (DFT) and path integral molecular dynamics (PIMD) to gain quantitative insight into biologically relevant systems. Our design of a better and more efficient approximation to quantum time correlation functions based on PIMD (TRPMD [1,2]) enables the calculation of ab initio TCFs with which we calculate IR/vibrational spectra and diffusion coefficients. In stacked polyglutamine strands (structures often related to amyloid diseases) a combination of NQE and H-bond cooperativity provides a small free energy stabilization that we connect to a softening of high frequency modes, enhanced by nuclear quantum anharmonicity [3]. [1] Rossi, Ceriotti, Manolopoulos, JCP **140**, 234116 (2014); [2] Rossi et al., JCP **141**, 181101 (2014); Rossi, Fang, Michaelides, JPCL **6**, 4233 (2015)

Mariana Rossi
University of Oxford

Date submitted: 06 Nov 2015 Electronic form version 1.4