Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

A Computational Study of Structural and Optical Properties in Model Crystal Structures of Amyloid Fibrils

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Hydrogen bonding pattern in fibrils

Fig. SI-1 below shows the hydrogen bond patterns in the fibrils obtained for 2Y3J similar to what was shown for 2Y2A in the manuscript in Figure 2.

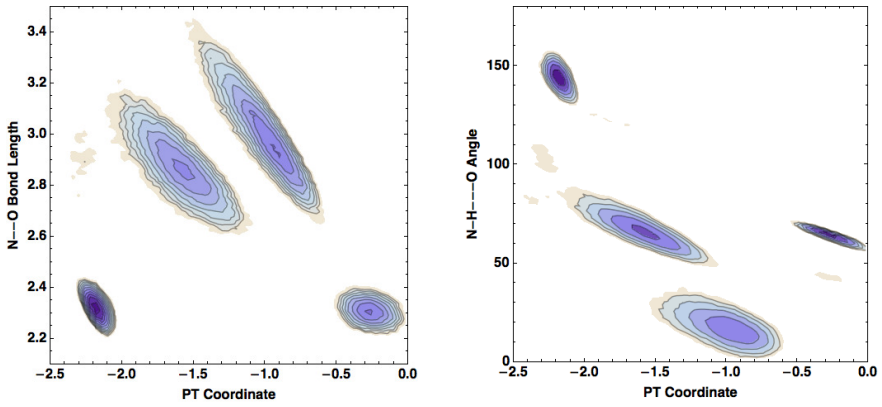

Figure SI- 1: 2D distributions of PT coordinate with respect to the N−O distance (left) and N−H−O angles (right), resulting from AIMD simulations on 2Y3J at 300K.

Potential Energy Surface Scans

In Fig. SI-2 we report examples of TD-DFT spectra, whose data are used to built the equivalent PES scans as in Figure from 5 to 8 in the manuscript. In Fig. SI-3 equivalent PES plot for 2Y2A along selected coordinate are also shown.

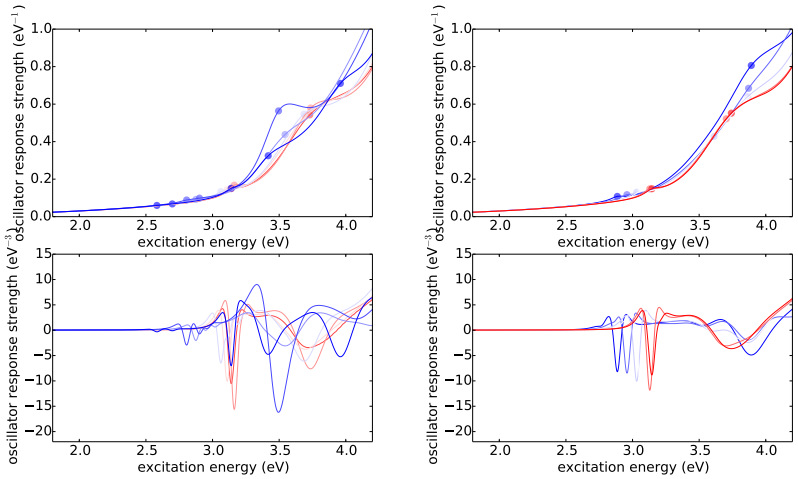

Figure SI- 2: Spectral evolution along PTC at N-C termini, in two cases where the proton is stabilized on the C-terminus (corresponding to displacement shown in Fig. 5 of the main article). Colors from red to blue qualitatively match the displacement from Oxygen to Nitrogen. The relevant steps along the PT coordinate and the corresponding PES are shown in Fig. SI-3 in left and middle panels, top sketches and bottom graphs respectively.

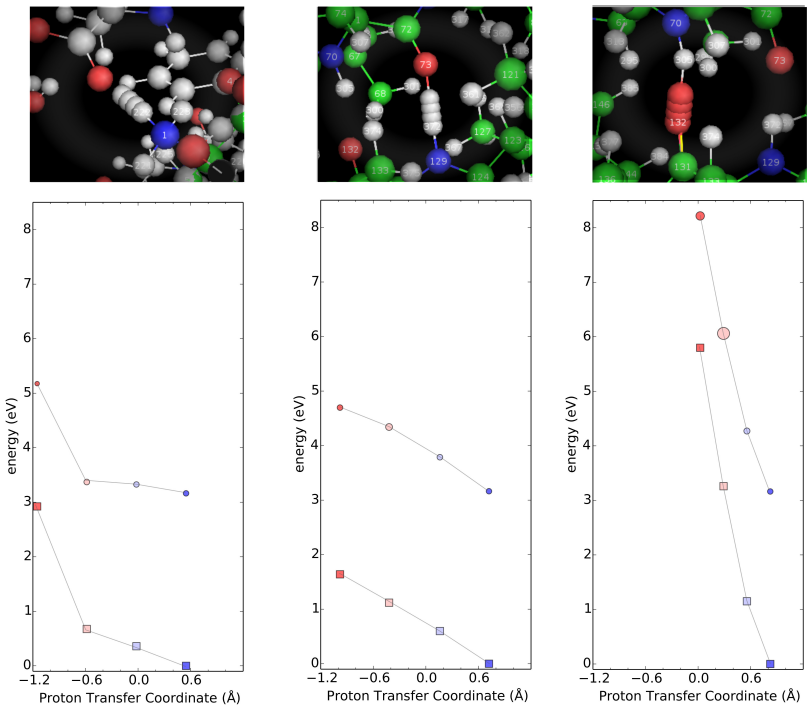

Figure SI- 3: 2Y2A ground and first excited-state PES on 0K equilibrium structure, along PTC in three cases: proton between N-ter and C-ter (left), from backbone N to opposite O (middle) and for C=O elongation. The size of circles for excited-state PES is proportional to the oscillator strengths of the transition. Colors from red to blue match the movement from Oxygen to Nitrogen, respectively. Figures on the top of each graph show the relevant steps along the PT coordinate, starting from equilibrium (solid atom sphere, colors red, white, blue and green correspond to Oxygen, Hydrogen, Nitrogen and Carbon respectively.).

AIMD: convergence information and sampling for spectra calculation

In Figures SI-4 and SI-5 we show examples of quantities extracted from the AIMD. Both shows that the timescales we are simulating allow us to make make definitive statements about quantities such as the populations of zwitterionic vs non-zwitterionic, or H-bonds patterns.

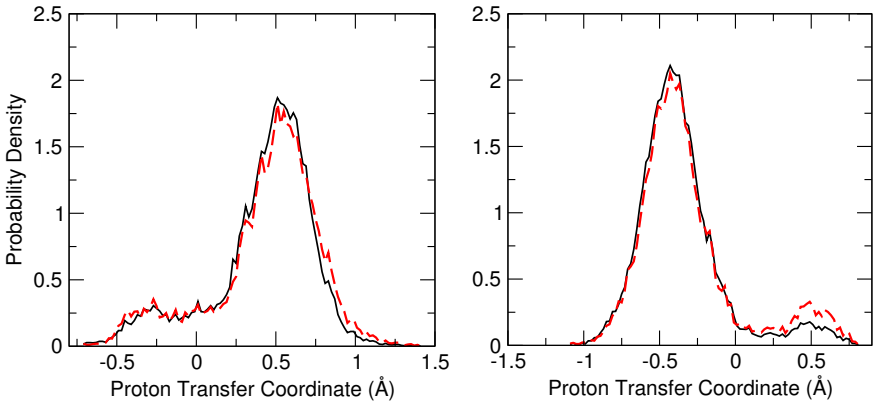

Figure SI- 4: Example of convergence on a relevant parameter: distribution probabilities along two selected proton transfer coordinate. Black line is obtained averaging over total length of the trajectory run, red dashed line is obtained only from the first half of the trajectory. The results do not differ significantly.

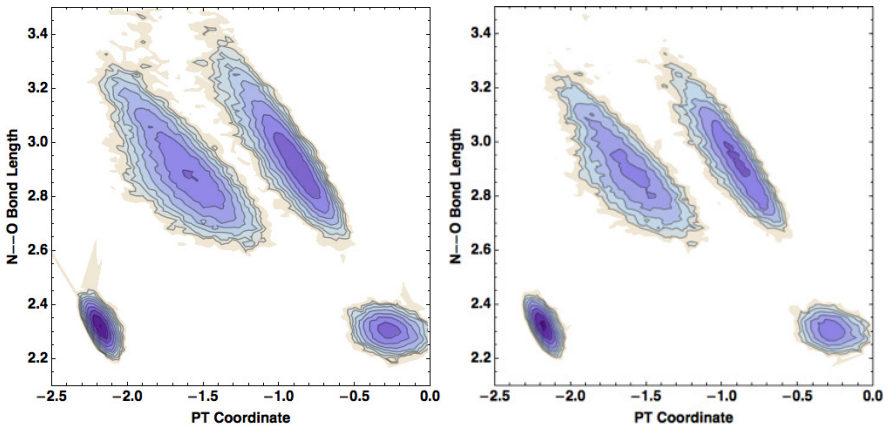

Figure SI- 5: Example of convergence on a relevant parameter: H-bonding pattern property, plotted as distribution respect to heavy atom length and angle. On the left the results is obtained averaging over total length of the trajectory run (same shown in a panel of Figure 2 of the main text) and on the right panel is obtained only from the first half of the trajectory. The results do not differ significantly.

We also report here a more detailed description of the procedure to obtain spectral data resumed in Fig. 10 in the main article. In particular, these are the computational protocols in details used to compute each spectrum (then averaged to get data in Fig. 10):

(a) averaging over all six NQE beads per time frame (from AIMD with PIGLET NQE)

(b) corresponding to a single NQE random bead per time frame (from AIMD with PIGLET NQE)

(c) averaging over three random NQE beads per time frame (from AIMD with PIGLET NQE)

(d) computed at the centroid coordinate per time frame (where the centroid is the averaged coordinate resulting from all 6 NQE beads, from AIMD with PIGLET NQE)

(e) computed at each time frame (from AIMD *classical nuclei*)

Even if obtained from two different simulations, results (d) and (e) are consistent and very similar (bottom panel in Figure 10).