**Figure S1.** The identity of the hydronium oxygen (bottom, black) and its nearest neighbor (top, red) during an exemplary 3 ps of BLYP and MS-EVB2 trajectories. Note that BLYP shows the “SP dance”, but not MS-EVB2, which exhibits many more successful PT events. Both trajectories show rapid fluctuations of the hydronium identity which are coupled, in the Zundel complex, to fluctuations in the identity of O$_{1x}$. 

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**SUPPORTING ONLINE MATERIAL:**

**Special Pair Dance and Partner Selection:**

**Elementary Steps in Proton Transport in Liquid Water**

Omer Markovitch, Hanning Chen, Sergei Izvekov, Francesco Paesani, Gregory A. Voth and Noam Agmon*
Figure S2. Equilibrium O–O radial distribution functions for the hydronium (black) and its first-shell neighbors (1x – red & 1yz – green) using all time-frames from BLYP and MS-EVB2 trajectories.
Figure S3. Conditional O—O radial distribution functions for the first solvation layer of the hydronium for trajectory segments of different lengths (indicated). From the long segments the first and last 50 fs were deleted. The RDFs for the Long intervals converge when their length > 300 fs. The RDFs for the Short intervals converge when their length <15 fs. These results depend only weakly on the water potential, even for diverse models such as MS-EVB3 and CPMD/HCTH.
Figure S4. Conditional O—O radial distribution functions for the hydronium using time-frames from long (blue) and short (cyan) trajectory segments from BLYP, MS-EVB2 and quantal MS-EVB3 trajectories. The yellow line shows a best fit to the equilibrium RDF (black, Fig. S2) using a linear combination of the two conditional RDFs with a factor $f = 0.74$ for BLYP and $f = 0.77$ for MS-EVB2. The fit did not succeed for the qMS-EVB3 trajectory.
Figure S5. Conditional O—O radial distribution functions for the hydronium nearest oxygen, O₁ₓ, using time-frames from long (blue) and short (cyan) trajectory segments from BLYP, MS-EVB2 and quantal MS-EVB3 trajectories. The yellow line shows a best fit to the equilibrium RDF (black, Fig. S2) using a linear combination of the two conditional RDFs with a factor $f=0.74$ for BLYP and $f=0.77$ for MS-EVB2. The fit did not succeed for the qMS-EVB3 trajectory.
Figure S6. The RDFs for Zundel and Eigen cations for various cutoff distances, $\Delta$ (in Å), in the geometric criterion of Marx et al. [23,41]. Our conditional RDFs for small and large non-transfer intervals are shown for comparison (black lines). The comparison shows that the best choice of cut-off distances is $\Delta_Z \leq 0.1$ Å and $\Delta_E = 0.2$ Å.
Figure S7. Time-dependent radial distribution functions for the hydronium [$g_0(r;t)$, in brown] and its nearest oxygen [$g_{1x}(r;t)$, in magenta] just before a proton hopping event in a HCTH simulation. The dashed and dotted lines show the same RDFs from the ensembles of long (Eigen, blue) and short (Zundel, cyan) trajectory segments. The larger noise for AIMD trajectories is due to their limited duration, dictated by their significantly greater computational cost.
Figure S8. Same as Figure S5 for an AIMD simulation with the BLYP functional.
Figure S9. Same as Figure S5 for a MS-EVB2 simulation.