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Determination of Protein Surface Hydration by Systematic Charge Mutations. JIN YANG, Department of Physics, The Ohio State University, MENGHUI JIA, State Key Laboratory of Precision Spectroscopy, East China Normal University, YANGZHONG QIN, Department of Physics, The Ohio State University, DIHAO WANG, Program of Biochemistry, The Ohio State Univeristy, HAIFENG PAN, State Key Laboratory of Precision Spectroscopy, East China Normal University, LIJUAN WANG, Department of Physics, The Ohio State University, JIANHUA XU, State Key Laboratory of Precision Spectroscopy, East China Normal University, DONGPING ZHONG, Department of Physics,Department of Chemistry and Biochemistry,and Programs of Biophysics, Chemical Physics and Biochemistry,The Ohio State University, DONGPING ZHONG COLLABORATION, JIANHUA XU COLLABORATION — Protein surface hydration is critical to its structural stability, flexibility, dynamics and function. Recent observations of surface solvation on picosecond time scales have evoked debate on the origin of such relatively slow motions, from hydration water or protein charged sidechains, especially with molecular dynamics simulations. Here, we used a unique nuclease with a single tryptophan as a local probe and systematically mutated neighboring three charged residues to differentiate the contributions from hydration water and charged sidechains. By mutations of alternative one and two and all three charged residues, we observed slight increases in the total tryptophan Stokes shifts with less neighboring charged residue(s) and found insensitivity of charged sidechains to the relaxation patterns. The dynamics is correlated with hydration water relaxation with the slowest time in a dense charged environment and the fastest time at a hydrophobic site. On such picosecond time scales, the protein surface motion is restricted. The total Stokes shifts are dominantly from hydration water relaxation and the slow dynamics is from water-driven relaxation, coupled with local protein fluctuations.

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