

Abstract Submitted
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Probing the water on chemically heterogeneous surface: interfacial-structural analysis for surface charge distribution SUCHEOL SHIN, ADAM WILLARD, Massachusetts Institute of Technology — We introduce the novel method for predicting the charge distribution of chemically heterogeneous surface, but reconstructed from the perspective of the interfacial water molecules. Our approach is to analyze the response of water to a disordered surface and infer from that response the heterogeneous distribution of surface charge. We accomplish this using a framework that is based on a probabilistic description of waters interfacial molecular structure and maximum likelihood estimation. This framework allows to deduce the apparent charge that is most congruently represented by the set of water configurations over the particular region of a surface. We demonstrate that the estimated charge distribution is consistent to the actual distribution for a static model substrate and hence that our method can be applied to investigate a dynamic fluctuating substrate such as the surface of a hydrated protein. This novel technique provides the useful information that can reflect the influence of fluctuations in the structure of biomolecule.

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