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Accurate thermodynamic computation of vibrational Stark shifts[1] ALISSA RICHARD, JOSE GASCON, Univ of Connecticut - Storrs — Vibrational Stark effect (VSE) spectroscopy allows for direct measurement of electric fields in biological systems, such as proteins, by utilizing a carbonyl or nitrile group as a vibrational probe. Because the probe's molecular vibrations are sensitive to non-covalent interactions of the environment, VSE spectroscopy provides an unique way to test the accuracy of electrostatic interactions in computational models. Here, we present research to address the challenges of quantifying electrostatic interactions as a thermodynamic average. Using realistic finite-temperature simulations, we quantify the relative electrostatic contributions of residues surrounding ketosteroid isomerase, and subsequently elucidate how inter-residue charge transfer as well as local and non-local polarization effects influence the electric field at the position of a molecular probe. In particular, we demonstrate that the inclusion of polarization effects and charge transfer are essential for a computational model to capture the correct thermodynamic structural average in comparison to experimental VSE spectroscopy.

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