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Title:Dipolar response of hydrated proteins
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Abstract:The paper presents an analytical theory and numerical simulations of the dipolar response of hydrated proteins in solution. We calculate the effective dielectric constant representing the average dipole moment induced at the protein by a uniform external field. The dielectric constant shows a remarkable variation among the proteins, changing from 0.5 for ubiquitin to 640 for cytochrome c. The former value implies a negative dipolar susceptibility, that is a dia-electric dipolar response and negative dielectrophoresis. It means that ubiquitin, carrying an average dipole of ≃240 D, is expected to repel from the region of a stronger electric field. This outcome is the result of a negative cross-correlation between the protein and water dipoles, compensating for the positive variance of the intrinsic protein dipole in the overall dipolar susceptibility. In contrast to the neutral ubiquitin, charged proteins studied here show para-electric dipolar response and positive dielectrophoresis. The study suggests that the dipolar response of proteins in solution is strongly affected by the coupling of the protein surface charge to the hydration water. The protein-water dipolar cross-correlations are long-ranged, extending ~2 nm from the protein surface into the bulk. A similar correlation length of about 1 nm is seen for the electrostatic potential produced by the hydration water inside the protein. The analysis of numerical simulations suggests that the polarization of the protein-water interface is highly heterogeneous and does not follow the standard dielectric results for cavities carved in dielectrics. The polarization of the water shell gains in importance, relative to the intrinsic protein dipole, at high frequencies, above the protein Debye peak. The induced interfacial dipole can be either parallel or antiparallel to the protein dipole, depending on the distribution of the protein surface charge. As a result, the high-frequency absorption of the protein solution can be either higher or lower than the absorption of water. Both scenarios have been experimentally observed in the THz window of radiation.
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