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Effect of the ordered interfacial water layer in protein complex formation: a non-local electrostatic approach ALEXANDER RUBINSTEIN, RENAT SABIRIANOV, University of Nembraska at Omaha — Using a non-local electrostatic approach that incorporates the short-range structure of the contacting media, we evaluated the electrostatic contribution to the energy of the complex formation of two model proteins. In this study, we have demonstrated that the existence of an low-dielectric interfacial water layer at the protein-solvent interface [1] reduces the charging energy of the proteins in the aqueous solvent, and consequently increases the electrostatic contribution to the protein binding (change in free energy upon the complex formation of two proteins). This is in contrast with the finding of the continuum electrostatic model, which suggests that electrostatic interactions are not strong enough to compensate for the unfavorable desolvation effects [2].

[1] Rubinstein and Sherman, Biophys. J. 87, 1544, 2004
[2] Rubinstein et al., Phys. Rev. E 82, 021915, 2010).

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