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Modeling Activity: Ions to Hydrophobics in Crowded Biological Solutions MONTGOMERY PETTITT, University of Houston — Nonideal solutions play a role in many aspects of chemistry. As concentrations increase, concentration itself becomes a less useful quantity to understand equilibria. Industrial and medicinal chemistry often fail due to the difference between concentration and activity. An understanding of the impact of the crowded conditions in the cytoplasm on its biomolecules is of clear importance to biochemical, medical and pharmaceutical science. Work on the use of small biochemical compounds to crowd protein solutions indicates that a quantitative description of their non-ideal behavior is possible and straightforward. Here, we will show what the structural origin of this non-ideal solution behavior is from expression derived from a semi grand ensemble approach. We discuss the consequences of these findings regarding protein folding stability and solvation in crowded solutions through a structural analysis of the mvalue or the change in free energy difference of a macromolecule in solution with respect to the concentration of a third component.

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