

Using DelPhi to compute saltation energy

In order to compute the saltation energy of a system at a given salt concentration two different DelPhi runs are required, first to compute the ΔG_z the energy of the system at zero salt concentration in the solvent and second to $\Delta G_{nz} ([\text{salt}])$, the energy at the given salt concentration [salt], here energy refers to grid energy of the DelPhi. Then saltation energy is $\Delta\Delta G_{nz} ([\text{salt}]) = \Delta G_{nz} ([\text{salt}]) - \Delta G_z$. In this section we will discuss two cases (I) saltation of a spherical charge whose analytical solution is also known and DelPhi results will be compared against analytical, and (II) saltation of a real protein (barnase-barstar complex).