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A Density Functional Theory of Transfer Free Energy in Protiens[1]

ERIC MILLS, STEVEN PLOTKIN, Dept of Physics & Astronomy, University of British Columbia — The cell environment in which proteins fold and function is crowded with biological molecules, at densities of ∼300g/L. Treating these molecules explicitly in a MD simulation introduces enormous computational cost, so accurate ways of modelling their contribution to protein behaviour is desirable. I will discuss existing models of transfer free energy (Auton and Bolen, Biochemistry 43, 1329) and solvation (Luchko et al, J Chem Thry Cmp it 6, 607) and propose a new approach, which uses classical density functional theory (Emborsky et al, Fluid Phase Equil 306, 15) to calculate the effect of these solutes on protein folding in a way that is efficient, yet accurate. The theory developed will be applied to both post-processing approaches and implicit solvent models.

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Eric Mills
Dept of Physics & Astronomy, University of British Columbia

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