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Solvation Free Energy and Classical Density Functional Theory[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 and propose a new approach, which uses classical density functional theory to calculate the effect of these solutes on protein folding. I will discuss implementing this approach as both an implicit solvent and a post-processing method, and discuss some general conclusions we can derive from it.

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

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