

# Relationship between solvation energy, chemical potential and hardness variations

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Starting from a density functional theory (DFT) formalism describing the energy change from one ground state representing an isolated solute, to another one representing the same solute in the field of the solvent, it is possible to obtain a simple and useful expression for the solvation energy in terms of the variation of the electronic chemical potential and global hardness associated to the change from gas to solution phase. Since both properties may be obtained from an orbital theory within the approximate Self Consistent Reaction Field (SCRF) methodology, the proposed model is expected to be useful for the analysis of chemical reactivity in solution.