

Density Functional Theory Applied to Liquids

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While density functional theory is known best for its applications to materials research, it also has been applied successfully to study condensed phases. In a biological system, water is the ever-present solvent and the fact that it participates in chemical reactions makes prediction of molecular properties difficult. Nevertheless, a realistic prediction of biological molecule activity will take into account the presence of water. We are developing ways to account for the effects of water on solute activity by coupling classical with quantum density functional methods, by coupling explicit with implicit methods, and by improving the implicit description of hydration.