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**A density functional approach for ab initio calculations in the presence of a solvent** JEAN-FRANÇOIS BRIÈRE, SAHAK PETROSYAN, DAVID ROUNDY, TOMÁS ARIAS, Department of Physics, Cornell University
— The study of a system in contact with liquid water typically involves a large number of atoms and averaging over a large number of configurations, making ab initio study of such systems prohibitive. This talk presents a formally exact way to circumvent this problem by separating the free energy of the system into three parts: a Kohn-Sham theory for the solute electron density, a classical density functional theory for the water molecular density, and a free energy of interaction between these two systems. We shall present various approximations for the interaction functional within this new joint density functional theory (JDFT) framework.

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