

Abstract Submitted
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Weighted density functional theory for water SAHAK PETROSYAN, DAVID ROUNDY, JEAN-FRANCOIS BRIERE, TOMÁS ARIAS, Cornell University — We report a weighted density functional theory for water that correctly describes bulk properties of water as well as perturbations at large and small length scales. Calculation of the free energy of solvation for hard sphere solutes of different sizes verifies that this functional gives a simple description of the hydrophobic effects in water. Use of this functional within a joint-density functional theory framework allows a rigorous replacement of molecular water with a continuum in Kohn-Sham calculations of systems in equilibrium with a solution.

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