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**The AM05 density functional applied to the water molecule, dimer, and bulk liquid** ANN E. MATTSSON, THOMAS R. MATTSSON, Sandia National Labs — We show that the AM05 exchange-correlation density functional (Armiento and Mattsson, Phys. Rev. B **72**, 085108 (2005)) yields a $H_2O$ dimer binding energy of 4.9 kcal/mol. The result is thus within 0.15 kcal/mol of CCSD(T) level theory ($5.02 \pm 0.05$ kcal/mol). We compare the AM05 results with those of five other functionals: LDA, PBE, PBEsol, RPBE, and BLYP. For liquid water, AM05 yields an O-O pair correlation function that is more structured than the ones of PBE and BLYP, which, in turn, are more structured than the one of RPBE. However, LDA and PBEsol yields more structured water than AM05. We confirm that accuracy in the water dimer binding energy is not a strong indicator for the fidelity of the resulting structure of liquid water. We will also report on the performance of AM05 for other systems and discuss the sub-system functional scheme used in the construction of AM05. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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