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Towards an accurate dissociative potential for water OMOLOLU AKIN-OJO, African University of Science and Technology, Km 10 Airport Rd, Galadimawa, Abuja, Nigeria — Most models of water describe the molecule as rigid, i.e., with fixed bond angles and bond lengths, or as flexible in which the bond angles and bond lengths vary but the chemical bonds cannot be broken. In this work we present our progress in the development of a water model which allows for the breaking and formation of chemical bonds. The force field was obtained by fitting *ab initio* (not DFT) energies, forces, and molecular properties. The ability of the model to predict properties of water at ambient and extreme conditions will be presented. We will also report on the modeling of small clusters of water using the dissociative force field.

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