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COMPUTATIONAL STUDY OF WATER CLUSTERS IN THEIR NEUTRAL AND ANION FORMS USING DENSITY FUNCTIONAL THEORY

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Abstract: Water is a molecule consisting of Hydrogen and Oxygen atoms with the molecular formula $(H_2O)n$, where n is the number of water molecules. Water is also the most abundant molecule on the earth's surface, most widely used universal solvent, and makes up an average of 60% of the human body making water an essential nutrient for all living organisms. Water clusters n = 2-10 has been studied using density functional theory (DFT) computational method MO6-2X paired with basis set 6-31+g(d) to observe their conformational changes, their interaction and adiabatic energies, and discuss their bond distances. The electrostatic potential map is also observed to understand the charge distribution difference when an electron is added to the neutral molecules. Results show an increase on the adiabatic energy for water clusters n = 6,8 suggesting these arrangements are more favorable. The interaction energy shows a decease linear line that is more uniform.