

Calculating Potential energy of a system of water molecules

The electrostatic, vanderwaal and total energy were calculated using the code. The outputs for the code are:

Total energy:	-4559.667472442094
Electrostatic Energy:	-5159.430611238769
Vanderwaal Energy:	599.7631387966753

electrostatic energy and vanderwaal energy was calculated for $^{432}\text{C}_2$ pairs of water molecules. It wasnt calculated for intramolecular atoms.