Abstract Submitted
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Electric-Field Induced Structural Evolution of Water Clusters $(H_2O)_n$ [n = 9 - 20]: *Ab initio* **Density Functional Approach**[1] RAJEEV PATHAK[2], Department of Physics, University of Pune, Pune, Maharashtra, India — Response of neutral water clusters $(H_2O)_n$, n = 9 through 20; to external electrostatic fields (0 to 1V/Å), is studied for the lowest-energy conformers within in the energy band ∼2 kcal/mol, for each "n," employing the versatile B3LYP hybrid prescription of density functional theory in conjunction with the polarized basis 6-311++G(2d, 2p). Increase in the field elongates and weakens hydrogen-bond networks; "opening up" three-dimensional cluster morphologies to complex net-like structures culminating into their disintegration at specific threshold values. All conformations are stable: they manifest as local minima on their potential energy surfaces. Field-induced structural transitions are invariably accompanied by an abrupt increase in the electric dipole moment, which is marked at breakdown, where the highest-occupied and lowest-unoccupied molecular orbital energy gap diminishes to zero. Remarkably, as a consequence of their zero or very small electric dipole moments, certain conformers endowed with molecular symmetry exceptionally exhibit a peculiar behavior: they either remain completely robust to increase in the field, or break up into smaller, identical, robust building units with tetramer, pentamer and hexamer ring- or cubic-geometries.

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