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Structural and Conductance Change in Hydridosilsesquioxane Based Silicon Oxide Clusters Induced by an Electric Field SAROJ NAYAK, PHILIP SHEMELLA, Rensselaer Polytechnic Institute - Department of Physics, Applied Physics & Astronomy — Interesting results arise from the addition of a hydrogen atom to a hydridosilsesquioxane (HSQ) $Si_8O_{12}H_8$ cluster, and have been studied with density functional theory techniques. Three stable minima have been found (open, cluster, center), and energy barriers between each have been computed. Each state has different values in the HOMO-LUMO[1] energy gap, which is usually a metric for conductance. Simulating the electronic interaction with an applied electric field, we model the reactions and compute the energy barriers with and without an applied electric field. Asymmetric states with strong dipole moments will have the most energetic effects in an applied field, based on the electric field-dipole energy relation, $U = -\mathbf{p} \bullet \mathbf{E}$.

We propose that the field forces the open structure to become energetically unstable, resulting in an overall loss in structures found in the open configuration and loss of the highly conducting properties. We have also modeled the critical energies points in implicit solvent, with results similar to gas phase calculations.

[1]Highest Occupied Molecular Orbital, Lowest Unoccupied Molecular Orbital

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