Structural and Conductance Change in Hydridosilsesquioxane Based Silicon Oxide Clusters Induced by an Electric Field

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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.

¹Highest Occupied Molecular Orbital, Lowest Unoccupied Molecular Orbital

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