Abstract Submitted
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Ab initio calculation of Stokes shifts of hydrogenated silicon clusters[1] MARIE LOPEZ DEL PUERTO, University of St. Thomas, St. Paul, MN, MANISH JAIN, University of California, Berkeley, CA, JAMES R. CHELIKOWSKY, University of Texas, Austin, TX — There is experimental evidence that hydrogenated silicon clusters may have large Stokes shifts. The absorption and emission processes in these clusters are not symmetric because the clusters may undergo structural changes while in an excited state. Several theoretical methods have been used to study this problem, resulting in an array of predicted Stokes shifts that differ in energy by several eVs, and different predicted minimum-energy structures with either relaxed cores or relaxed outer shells. We calculate Stokes shifts using three different methods: density functional theory within the local density approximation (LDA), density functional theory within the generalized gradient approximation (GGA), and time-dependent density functional theory within the local density approximation (TDLDA). We find that these three different methods give similar results both for magnitude of Stokes shift and excited-state structures. The Stokes shift of hydrogenated silicon clusters of 5 to 35 silicon atoms range from 5.5eV to 0.8eV, decreasing with increasing cluster size.

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