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Calculated Polarizabilities of Diamond and Silicon Nanoclusters[1]

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— A scheme for decomposing the electric polarizability of a system into site-specific contributions is applied to hydrogenated nanoclusters of carbon and silicon. Site-specific dipole moments and polarizabilities are obtained from the response of charge densities to external electric fields, and decomposed into local and charge transfer components. We study changes in the polarizabilities of the C and Si atoms as the clusters grow in size. We find that exterior atoms have larger polarizabilities than interior atoms and that the charge transfer contribution to the total cluster polarizability increases with cluster size. We examine the relationship between the atomic polarizabilities in these clusters and bulk polarizability in carbon and silicon.

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