Title:	Enhanced CO2 adsorption on doped Au32 gold nanocages: A density functional approach
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Abstract:	The properties of Au32 clusters through selective doping with Si, Ge and Cu atoms and its interaction with CO2 molecule are reported in this work. The relative stabilities of the clusters compared on the basis of average binding energy per atom indicated that Cu12Au20 is stable with a binding energy of −86.085 kcal mol−1/atom. A charge density-based analysis of the doped clusters is also presented. The highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) energy gap of M12Au20 cluster (M denotes dopants) is much smaller, compared to that of the Au32 cluster, implying higher reactivity. Molecular electrostatic potential (MESP) and its analysis gave guidelines to the various possible sites for the adsorption of CO2 molecule. The most favourable dopant for CO2 adsorption was found to be Cu amongst all the others. Calculated Infrared (IR) frequencies indicate that Cu-doped gold clusters give maximally intense peaks for CO2 stretching. Absorption spectra of the nanocages are also presented using time-dependent density functional theory (TDDFT). This has maximum change in wavelength for Si-doped cluster on CO2 adsorption. The structural and band gap changes are manifested in the catalytic properties with the result that the doped cages showed strong adsorption for CO2 as compared to pristine Au32 cluster, with Cu being the best doping agent.
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