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Density Functional Study of Strain Effects on the Energy Gap in Silicon Nanoclusters XIHONG PENG, AZAR ALIZADEH, NITIN BHATE, SURYA GANTI, GE Global Research, Niskayuna, NY 12309, PRADEEP SHARMA, Department of Mechanical Engineering, University of Houston, Houston, TX 77204, SAROJ NAYAK, SANAT KUMAR, Departments of Physics and Chemical Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180 — It is well known that nanoscale Si clusters are photo luminescent. In parallel, industry routinely exploits the dramatic strain dependence of the band gap of bulk Si for electronics applications. We have discovered, using density functional calculations that the combined role of finite size and strain leads to previously unanticipated effects on the energy gap in Si clusters. Both hydrostatic and non-hydrostatic strains were applied to the clusters with sizes up to 2nm. For the hydrostatic strain, which maintains the tetrahedral bonding network in Si, the effects of strain on the energy gap exhibits size dependence. The behavior can be classified in three distinct regimes that will be discussed in detail. For non-hydrostatic strains, which result in distortion of the tetrahedral bonds, the coupling between the energy gap and strain is largely independent of the cluster size. The mechanisms responsible for the coupling between the gap and strain are proposed. The relative shifts of the energy gap for hydrostatic and non-hydrostatic strains are compared.

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