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The effect of polytype on energy gap in SiC nano-clusters XIHONG PENG, AZAR ALIZADEH, NITIN BHATE, LARRY ROWLAND, GE Global Research, Niskayuna, NY 12309, SAROJ NAYAK, SANAT KUMAR, Departments of Physics and Chemical Engineering, Rensselaer Polytechnic Institute, Troy, NY 12810 — The size dependence of energy gap is perhaps the most remarkable aspect of quantum confinements in low dimensional systems. Numerous models have been proposed to describe the quantum confined electronic states in Si, CdSe, etc, providing a precise description of the bandgap as a function of nano-crystal dimensions. Recently, ab-initio studies of energy gap in cubic SiC nanoparticles as a function of both size and surface composition have been reported. SiC is a remarkable semiconductor with over 200 different crystal structures (polytypes) due to different stacking orders. The always-indirect band gap of bulk SiC varies substantially among the different polytypes (2.4 eV for 3C-SiC to 3.3 eV for 2H-SiC). We have investigated the effect of polytypism on the size-dependency of energy gap in SiC nano-clusters using ab-initio calculations. For clusters smaller than 1 nm, all SiC polytypes show identical energy gap-size dependencies. For SiC nano-particles larger than 1 nm, the effect of crystal structure becomes apparent approaching the bulk values.

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