A Quantitative Understanding of Ge Hut Formation on Si(001) Surface from First-principles[1] GUANG-HONG LU, N.-Y. MA, FENG LIU, Department of Materials Science & Engineering, Univeristy of Utah, MARTIN CUMA, Center for High Perfomance Computing, Univeristy of Utah — Ge growth on Si(001) is characterized by layer-by-layer growth, followed by 3D island formation with a distinct initial island shape of "hut" bounded by (105) facets. Despite of extensive studies over the last decade, our understanding of hut formation remains qualitative that it forms by strain relaxation overcoming the cost of increased surface energy but the values of strain energies and surface energies are unknown. We have carried out extensive first-principles calculations to determine, respectively, the surface energies and stresses of Ge/Si (001) and (105) surfaces and their strain dependence as a function of Ge coverage. Using these as inputs to continuum theory, we provide a quantitative analysis of Ge hut formation on Si(001).

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