Structure competition in growth of In island on Si111 from first-principles calculations CAI-ZHUANG WANG, MIN JI, J. CHEN, M. HUPALO, M.C. TRINGIDES, K.M. HO, Ames Laboratory US-DOE and Department of Physics, Iowa State University, Ames, IA 50011, USA — We have carried out first principles calculations to understand the growth of indium island on Si111 substrate which have been observed to have an interesting FCC and BCT structure competition. Our calculations show that quantum size effect (QSE) plays an important role in different island structure formation. Furthermore, the interface energy between In and Si substrate also controls the relative stability of different island structures.

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