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Density Functional Study on Energetic Instability of the 5×2 structure on Au/Si(111) and Au/Si(775) surfaces. MASASHI NODA, TAKUYA KADOHIRA, SATOSHI WATANABE, Dept. of Materials Engineering, The University of Tokyo and CREST-JST, CHRIS FISCHER, GERBRAND CEDER, DMSE, Massachusetts Institute of Technology — Atomic configurations of Au/Si(111) surface have been examined extensively. However, there are only few systematic theoretical analyses taking account of the variation of Au and Si coverages. Keeping this in minds, we have done such a systematic analysis on the energetic stability of various models proposed for Au/Si (111) structures so far using density functional calculations. As a result, we obtained good agreement with experimental results on the periodicity of energetically stable structures except that none of the models with 5×2 periodicity are predicted to appear in our calculation. Then, we examined the possibility of stabilizing some of the 5×2 models by the effects of steps, using Au/Si(775). We found that none of the 5 ×2 structures are stable even on Si(775). These results suggest that we have to explore a new model to explain the observed 5×2 structure.

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