J. Appl. Phys. **110**, 064314 (2011); http://dx.doi.org/10.1063/1.3638071 (*6 pages*)

Formation of nanoscale gold chain on a Si(110) surface: A density functional investigation

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(Received 27 May 2011; accepted 7 August 2011; published online 22 September 2011)

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The adsorption of gold (Au) atoms on a Si(110) surface is theoretically investigated by employing the first-principles plane wave pseudopotential method and the density functional scheme. We have examined the atomic geometries of stable atomic Au wire formation, leading to (1×2) and (2×5) reconstructions of the Si(110) surface, corresponding to the Au coverages of 0.25 monolayer and 0.4 monolayer, respectively. Both reconstructions are found to have metallic nature, with at least two dispersive bands crossing the Fermi level. The effective mass values of the near-Fermi bands are estimated and compared with the available experimental findings.

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Keywords

ab initio calculations, adsorption, density functional theory, effective mass, elemental semiconductors, Fermi level, Fermi surface, gold, monolayers, pseudopotential methods, silicon, surface reconstruction

PACS

71.15.Mb
Density functional theory, local density approximation, gradient and other corrections

71.18.+y
Fermi surface: calculations and measurements; effective mass, g factor

68.35.bg
Semiconductors

68.43.Bc
Ab initio calculations of adsorbate structure and reactions

68.43.Mn
Adsorption kinetics

71.15.Dx
Computational methodology (Brillouin zone sampling, iterative diagonalization, pseudopotential construction)

ARTICLE DATA

Digital Object Identifier

http://dx.doi.org/10.1063/1.3638071

PUBLICATION DATA

ISSN

0021-8979 (print)
1089-7550 (online)

Publisher

American Institute of Physics

crossref Member

For access to fully linked references, you need to log in.

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