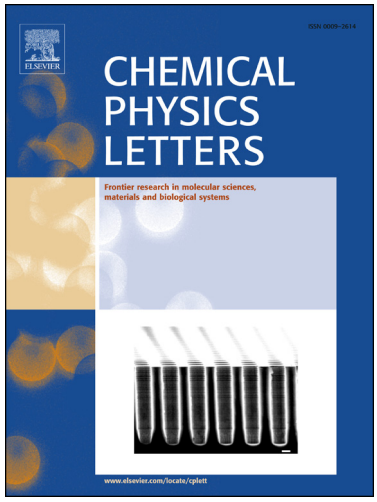

Bandgap opening in silicene: effect of substrates

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PII: S0009-2614(13)01517-0
DOI: http://dx.doi.org/10.1016/j.cplett.2013.12.036
Reference: CPLETT 31828

To appear in: *Chemical Physics Letters*

Received Date: 24 October 2013
Accepted Date: 16 December 2013

Please cite this article as: N. Gao, J.C. Li, Q. Jiang, Bandgap opening in silicene: effect of substrates, *Chemical Physics Letters* (2013), doi: http://dx.doi.org/10.1016/j.cplett.2013.12.036

Bandgap opening in silicene: effect of substrates

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Abstract

Our density functional calculations show that opening a sizeable band gap of silicene without degrading its carrier mobility can be realized by silicene-substrate hybrid structures with noncovalent interface interactions. Several possible two-dimensional semiconducting substrates are selected to find the factors that control the magnitude of band gap. It is found that the more notable charge redistribution in two sublattices of silicene and thus a larger band gap is characterized by a smaller interlayer distance. Thus, the opened band gap in hybrid structures with SiH/π interaction has reached the technique requirement of room-temperature operation in field effect transistors.

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