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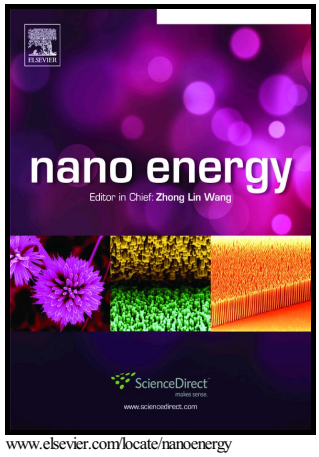

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Abstract

Crystalline silicon is dominating the current solar cell market due to the significant efficiency improvement and cost reduction in last decades. However, its indirect band gap nature leads to inefficient visible-light absorption, which seriously impedes further performance enhancement in silicon-based photovoltaic devices. Thus, it is highly desirable to develop direct band gap silicon materials. Herein, by means of ab initio swarm-intelligence structure-searching method, we predicted a quasi-direct gap semiconducting tri-layer silicene structure consisting of alternating arrays of six-membered Si rings, which can be converted into a