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Si3AlP: A New Promising Material for Solar Cell Absorber JIHUI YANG, YINGTENG ZHAI, HENGRUI LIU, HONGJUN XIANG, XINGAO GONG, Fudan University, SUHUAI WEI, National Rewable Energy Laboratory — First-principles calculations are performed to study the structural and optoelectronic properties of the newly synthesized nonisovalent and lattice-matched (Si2)0.6(AlP)0.4 alloy [T. Watkins et al., J. Am. Chem. Soc. 2011, 133, 16212.] The most stable structure of Si3AlP is a superlattice along the <111>direction with separated AlP and Si layers, which has a similar optical absorption spectrum to silicon. The ordered C1c1-Si3AlP is found to be the most stable one among all the structures with –AlPSi3- motifs, in agreement with the experimental suggestions. We predict that C1c1-Si3AlP has good optical properties, i.e., it has a larger fundamental band gap and a smaller direct band gap than Si, thus it has much higher absorption in the visible light region, making it a promising candidate for improving the performance of the existing Si-based solar cells.

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