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A New Silicon Allotrope with a Direct Band Gap for Optoelectronic Applications YAGUANG GUO, QIAN WANG, Peking University, YOSHIYUKI KAWAZOE, Tohoku University, PURU JENA, Virginia Commonwealth University, PEKING UNIVERSITY TEAM, KAWAZOE COLLABORATION, JENA COLLABORATION — Silicon structures with direct band gaps have been hotly pursued for solar cell applications. To effectively harvest the sunlight in the whole frequency region, it is a good strategy to use arrays consisting of Si structures with different direct band gaps. However, the structure with a direct band gap about 0.6 eV has been missing according to current progress made in the direction. Here we report our findings that the missing structure can be constructed by using Si triangles as the building blocks, which is stable dynamically and thermally, not only exhibiting the desirable band gap, but also showing high intrinsic mobility and low mass density. These advantages over the existing Si structures would motivate new experimental effort in this direction.

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