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Exceptional Optoelectronic Properties of Si-related compounds

BING HUANG, HOULONG ZHUANG, MINA YOON, ORNL, SU-HUAI WEI, NREL, BOBBY SUMPTER, ORNL — The search of new silicon-related functional compounds are of great interests but still very changeling. In the last few decades, researchers have heavily studied the structural and electronic properties of silicon in order to improve its optical absorption in the visible light range using analyses of metastable silicon phases, silicon-based alloys, and silicon-based superlattices. In this talk, I will present our recent theoretical efforts on searching and designing new silicon phases, from bulk to two-dimensional (2D) silicon, with exceptional optoelectronic properties. Especially, we find that chemically functionalized 2D silicon and silicon alloys could be the best candidates to create efficient thin-film solar absorbers and silicon-based, white-light-emitting diodes, paving the way for new “green” energy applications.

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