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Theory of hydrogen related meta-stability in disordered silicon[1]
BLAIR TUTTLE, Penn State Erie — Density functional electronic structure calculations are employed to examine hydrogen for a variety of configurations in silicon. A novel complex is found for hydrogen in amorphous silicon. The complex involves the breaking of weak silicon bond to form two Si-H bonds with both hydrogens in between the original silicon atoms. This complex provides a microscopic model for new metastable complexes observed in amorphous silicon. Mechanisms for hydrogen-related metastability will be discussed for amorphous and ppoly-crystalline silicon.

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