

Formation of clean dimers during gas-source growth of Si(001)

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Elevated temperature STM measurements have shown that one key phase during gas-source homoepitaxy of Si(001) is the formation of clean Si ad-dimers from hydrogenated ad-dimers, though the mechanism for this formation is unknown. We present *ab initio* density functional calculations designed to explore this mechanism. The calculations show that there is a pathway consistent with the experimentally observed reaction rates, which proceeds via a meta-stable intermediate, and is effectively irreversible. This result fills a vital gap in our understanding of the atomic-scale details of gas-source growth of Si(001).