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First-principles studies of isomerization processes of silicon clusters LEONIDAS TSETSERIS, GEORGE HADJISAVVAS, SOKRATES PANTELIDES, Vanderbilt University — Nanoclusters typically exhibit a large number of isomers, often with strikingly different structural and electronic properties. Controlled growth and use of these ultrasmall particles depends, therefore, on an understanding of the atomic-scale details of inter-isomer conversions. Here we use first-principles calculations to study the isomerization kinetics of silicon clusters. Based on the results on activation energies, we infer a classification scheme for the complex phase of isomers in domains which are delineated by bond-breaking events at the outer cluster shells. Our findings are consistent with experimental measurements and they have implications for theoretical searches of low-energy cluster structures. We also present results on hydrogenation and oxidation kinetics and we discuss their relevance for pristine and functionalized silicon clusters. This work was supported in part by DOE Grant DEFG0203ER46096.

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