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Quantum Monte Carlo Studies of Buckling of the Si(100) Surface WENDY LAMPART, RICHARD CHRISTIE, DANIEL SCHOFIELD, KENNETH JORDAN, University of Pittsburgh Department of Chemistry — The quantum Monte Carlo method is used to study the role of electron correlation on the buckling of Si-Si dimers on the Si(100) surface. The buckling is addressed using cluster models with one to three surface dimers. In addition to the diffusion Monte Carlo method, calculations are also carried out using various density functional methods, multi-reference MP2, multi-reference MP3, and approximate multi-reference coupled cluster approaches. The calculations show that high-order correlation effects are important for determining the relative stability of the buckled and unbuckled structures, favoring the buckled structure.

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