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Structure and Dynamics of Silicon Carbide Clusters: A Tight-Binding Adaptive Monte Carlo Application ANTHONY PATRICK, XIAO DONG, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 22030, THOMAS ALLISON, ANWAR HASMY, National Institute of Standards and Technology — A tight-binding parametrization for silicon carbide nanoclusters was developed based on the electronic energy surface of small clusters calculated within the generalized gradient approximation of density functional theory. This parametrization includes s and p angular momentum symmetries and parameters for the on-site, hopping and overlap matrix elements. With the aid of these new parameters, the global minima of silicon carbide clusters in the range of 10-30 atoms were discovered with the adaptive Monte Carlo Method [1]. The ATMC optimization process is fast and drives the system across configuration space very effectively reaching the global minimum in a small number of tempering events. Growth sequence, stability patterns, and temperature behavior were also obtained. [1] X. Dong and E. Blaisten-Barojas, J. of Comp. & Theor. Nanoscience, 3, 118-127 (2006).

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