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First-principles calculations of low coverage growth of Ba on Si(001) C. R. ASHMAN, High Performance Technologies Inc., C. J. FOERST, P. E. BLOECHL, Clausthal University of Technology, DOD HPCMP PET PROGRAM COLLABORATION, CLAUSTHAL UNIVERSITY OF TECHNOLOGY, INSTITUTE FOR THEORETICAL PHYSICS COLLABORATION — Ba is of interest to the semiconductor industry for it's possible use in replacement gate oxide materials and for possible use in a buffer layer between Si(001) and Ba containing dielectric materials. Thus it is of importance to understand the initial stages of growth. This paper reports state-of-the-art electronic structure calculations on the deposition of Barium on the technologically relevant, (001) orientated silicon surface. We identify the surface reconstructions from zero to one monolayer and relate them to previous theoretical studies of low coverage Ba growth and Sr growth.

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