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**Structural and Electronic Properties of Boron Doped Multiply Twinned Silicon Nanowires** C.S. JAYANTHI, PAUL TANDY, M. YU, S.Y. WU, University of Louisville, Y. ZHAO, NREL, UNIVERSITY OF LOUISVILLE/NATIONAL RENEWABLE ENERGY LAB COLLABORATION — Previous studies of undoped multiply twinned (MT) silicon nanowires (SiNWs) have found these structures to be more stable than the bulk-cut single crystal SiNWs for diameters $< 6$ nm [1]. The five segments that form the MT-SiNWs result in a strain field, causing the interior region of the MT-SiNW to compress while stretching its exterior. In fact, the distribution of the internal stress field in MT-SiNWs offers a unique opportunity for doping the MT-SiNW, including bi-polar doping, and thus opening doors to novel designs of photovoltaic elements. In this work, we will use highly efficient quantum mechanical simulations based on the semi-empirical Hamiltonian developed in Ref. [2] to investigate the electronic structure of boron doped MT-SiNWs of different diameters. We will first determine the most favorable locations for placing boron atoms by mapping out the stress fields of undoped MT-SiNWs. To understand the doping characteristics, we will compare the local site energies and local electronic density of states of MT-SiNWs of undoped and doped systems, and carry out the calculation for MT-SiNWs of different diameters. 1. Y. Zhao, Phys. Rev. Lett., 91, 035501 (2003). 2. C. Leahy *et al.* Phys. Rev. B74, 155408 (2006).

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