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Atomic Structure of the Si(111)-4x1-In System[1] BARRY HAYCOCK, West Virginia University & Dublin Institute of Technology, J.D. O'MAHONY, Dublin Institute of Technology — The indium-induced 4 x 1 reconstruction on silicon (111) has been extensively studied due to its unique physical structure and electronic properties, which indicate so-called "Quantum Wire Behaviour". The likely crystallographic structure of this system has been hotly debated since 1999. The structure was mathematically modeled by Tsay using a planewave calculation method in 2005, which yielded results of atomic positions that matched closely to the Bunk model. In this study we model the this system using the molecular dynamics (MD) package Fireball, taking as a starting point the atomic positions of the Bunk model. This ab-initio tight-binding MD method has the advantage of being able to operate with a very large number of atoms per cell in a single calculation, thus allowing for a very large superslab in the calculation model. This allows for greater surface area and thus is expected to produce a more accurate surface characteristic calculation result. The results of this calculation are compared to the recent results of Tsay.

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