

Abstract Submitted
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Ab Initio Studies of Indium Diffusion on the Si(111)-7x7/Ge(111)-5x5 Surface¹ D. PSIACHOS, Dept. of Physics, Queen's University, M. J. STOTT, Dept. of Physics, Queen's University — The mechanisms for the self-assembly of ordered arrays of indium magic clusters on the Si(111)-7x7/Ge(111)-5x5 surface have been investigated theoretically using ab initio total energy simulations. Plane wave density functional methods have enabled us to obtain the potential energy surface for one indium atom adsorbed on the Ge(111)-5x5 surface. Using these ab initio-derived energies as input, a classical molecular dynamics simulation has yielded values for the temperature-dependent, trajectory-dependent, microscopic self-diffusion coefficients of an indium atom on the Ge(111)-5x5 surface. For comparison, we also have calculated the diffusion coefficient obtained through fully ab initio molecular dynamics where we have used the non-self-consistent Harris Functional due to computational cost. Also, as a third approach, the harmonic approximation of the transition state theory has been applied and is assessed in light of the two molecular dynamics simulations. The single-atom results show promise for providing useful information on how the magic clusters on semiconductor surfaces may be formed.

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