

Abstract Submitted
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Multi-step atomic interchange mechanism for atom manipulation on semiconductor surfaces. BATNYAM ENKHTAIVAN, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo — We report on our total-energy electronic-structure calculations based on the density-functional theory that clarify atom-scale mechanisms of atom-manipulation recently realized on semiconductor surfaces [1]. We focus on Ge(111) and Si(111) surfaces and identify reaction pathways and corresponding reaction energy barriers. Considering the atom manipulation of Pb and Sn atoms on Ge(111) surfaces, we find that the substitutional Sn (Pb) diffuses to neighboring Ge adatom, and forms a dimer with Ge spontaneously. Then the Sn (Pb) and the Ge adatom exchange their position concertedly with the dimer structure kept. These diffusion and exchange processes are multi-step atomic processes consisting of multiple metastable states. For the case of Sb manipulation on the Si(111) surface, the dimer structure does not form spontaneously when the AFM tip is absent. We find that the roles of the AFM tip during the atom manipulation are the lowering of the diffusion energy barrier and stabilization of the dimer structure. [1] Y. Sugimoto et al., e-J. Surf. Sci. Nanotech. 4, 376-383 (2006).

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