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First principles study of Atomic Force Microscope manipulation of Ag atom on Si(111)-(7x7) surface. BATNYAM ENKHTAIVAN, ATSHUSHI 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 Si(111)-(7x7) surface at room temperature [1]. We focus on Ag adatom diffusion between the half unit cells (HUC) of Si(111)-(7x7), and identify reaction pathways and corresponding reaction energy barriers. We have found three different reaction pathways. Without the presence of the AFM tip, the rate determining barrier is 0.8 eV. We consider the manipulation by the Si and Pt tips. When the tip-surface distance is 3.5 angstrom, due to the interaction between the tip and the diffusing adatom, the reaction barrier is reduced to about 0.25 eV and 0.60 eV by Si and Pt tips, respectively. We find that the reduction of the barrier depends on the flexibility of the tip apex structure. The tip apex adatom of Si tip moves about 0.86 angstrom toward Ag adatom to form bond, while that of Pt tip does not move. The tip not only reduces the diffusion barrier, but also traps the adatom under it. We find that the shape of the tip apex is important. When the adatom interacts with multiple tip atoms, the adatom is strongly trapped. [1] Y. Sugimoto et al., Nat. Commun. 5, 4360 (2014).

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