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Theoretical Study on F atom diffusion on Si(111) surface NARA JUN, National Institute for Materials Science and Institute of Industrial Science, University of Tokyo, YUSUKE ASARI, National Institute for Materials Science, TAKAHISA OHNO, National Institute for Materials Science and Institute of Industrial Science, University of Tokyo — We studied diffusion mechanisms of fluorine atom adsorbed on Si(111) surface in a low coverage regime by means of the first-principles density functional calculation. Recent experiments found that the diffusion frequency of the fluorine atoms on Si(111)-(7x7) surface is very low and interestingly it is enhanced after the deposition of silicon atoms on the surface. While this measurement strongly suggests that the diffusing extra silicon atoms assist the fluorine migration, the mechanism has not been understood yet. We found that it is hard for F atoms to hop between surface Si atoms directly because of the strong Si-F bonding. Instead we suggest the SiF complex diffusion model, in which SiF bond is kept during diffusion. This model is also understood as the Si atom diffusion with carrying the F atom. This model, in which the activation energy is calculated to be 1.34 eV, can explain the experiment very well. This work was partly supported by RSS21 project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.

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