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First-principles study of the Br/Si(100) surface

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The interactions of Si(100) with halogens have been widely investigated because of the importance of halogen etching in fabrication of semiconductor devices. Recently, Nakayama and co-workers have studied tunneling electron induced Br hopping on Si(100)-(2x1) by scanning tunneling microscopy (STM).(1) They argued that Br hopping can be accomplished through a combination of electron capture in Si-Br antibonding levels and inherent adsorbate repulsive interactions. To understand these experimental results, first-principles total-energy and electronic structure calculations are necessary.

We present the results of pseudopotential density-functional calculations for the Br/Si(100) surface. The calculated bonding geometries, surface band structures, and simulated STM images will be compared with experiments.

[Reference]
1. K. S. Nakayama, E. Graugnard, and J. H. Weaver, Phys. Rev. Lett. 89, 266106 (2002).