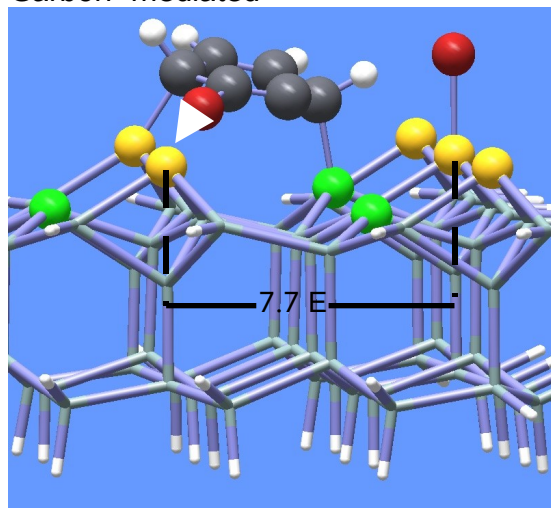


## Nanoscale patterning on a Si(111) surface

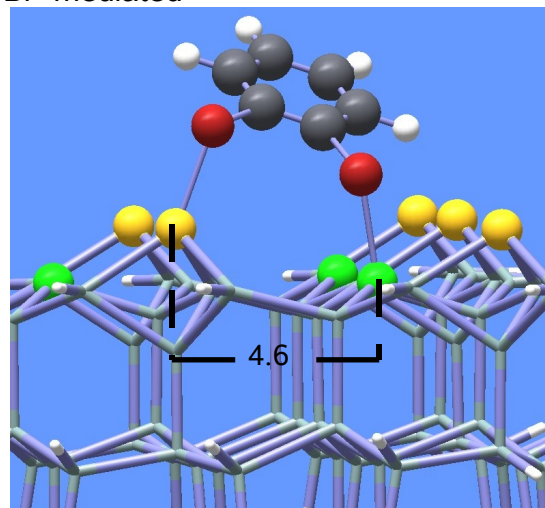
Reactions of molecules with surfaces of Si have been of particular interest as a means to the chemical modification of these surfaces, in view of the great importance of Si in the field of microelectronics technology. For example, bromination of Si(111) by 1,2- and by 1,4- dibromobenzene leads to different patterns. <http://www.utoronto.ca/jpolanyi/science/science6.pdf>

### Reaction of 1,2-dibromobenzene at Si(111)

Carbon- mediated

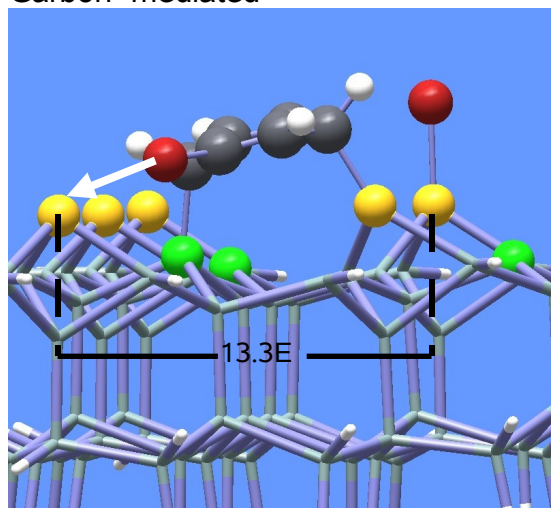


Br- mediated

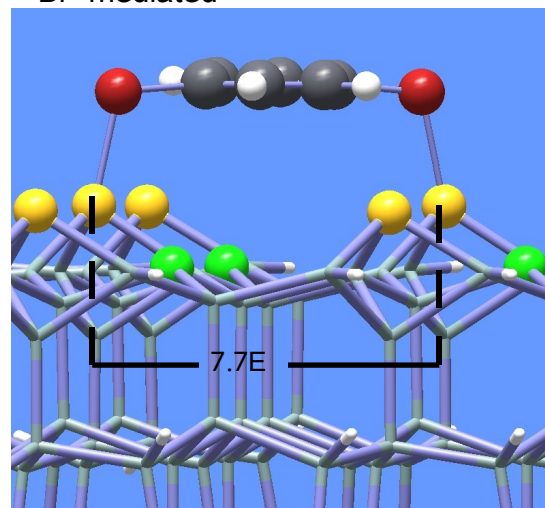


### Reaction of 1,4-dibromobenzene at Si(111)

Carbon -mediated



Br- mediated



At TPCI, we employ AM1 and DFT methods to calculate geometries, energies and reaction paths of physisorbed and chemisorbed organic molecules at Si(111).[references 1- 4]

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- [2] K. Rajamma Harikumar, Ioannis D. Petsalakis, John C. Polanyi, and Giannoula Theodorakopoulos, Theoretical study of the halogenation reactions of 1,2- and 1,4-dibromobenzene at Si(111)-7×7, Surface Science 572 162 (2004)  
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- [3] I.D.Petsalakis, J.C.Polanyi and G Theodorakopoulos, Theoretical study of benzene, toluene and dibromobenzene at a Si(111)7X7 surface. Israel Journal of Chemistry (in press,2005)
- [4] I.D.Petsalakis and G Theodorakopoulos, Theoretical study of halogen-substituted benzene at a Si(111)7X7 surface. Israel Journal of Chemistry (in press,2005)