Energy Scaling and Surface Patterning of Halogen-Terminated Si(001) Surfaces $^1$ DUANE D. JOHNSON, NIKOLAI ZARKEVICH, Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — We show that the steric repulsion energies between halogen dimers on a passivated Si(001) surface scale with square of the principle quantum number of the halogen, and arise mostly from bonding with Si substrate. We exemplify the scaling from previously calculated steric interactions of F, Cl, and Br, predict the interactions for I and At, and verify the prediction by density-functional calculations. From the energetics, we explain the patterning of the halogen-terminated Si(001), providing a better understanding of the halogen-roughening process, and predict a crossover to a new vacancy-line defect for large halogens.

$^1$Work is supported by NSF (DMR-0325939), and the DOE (DEFG02-91ER45439) at the Frederick Seitz Materials Research Laboratory.