Relative stability of Si surfaces: a first-principles study\textsuperscript{1} GUANG-HONG LU, MINGHUANG HUANG, FENG LIU, Department of Materials Science and Engineering, University of Utah, MARTIN CUMA, Center for High Performance Computing, University of Utah — Surface energies of solid surfaces are often calculated by the supercell slab technique subtracting the bulk energy from the total energy of supercell. However, there exists a common mistake that the same bulk atom energy obtained by a separate bulk calculation is used for different surface orientations and slab sizes, which makes the surface energies divergent and the comparison of their relative stability unreliable. The more accurate way to determine the atom bulk energy is to extract the atom bulk energy and surface energy simultaneously by fitting slab total energy as a function of atom number in the slab. Here, using this method, we have calculated surface energies of Si (001), (110), (111), and (113) surfaces with different reconstructions systematically using first-principles total-energy method. The relative stability of these Si surfaces are shown in decreasing order as (111), (001) to (113) at low temperature, and (001), (113), (110) to (111) at high temperature, respectively. Si(113) is found to be a stable surface at both high and low temperature in spite of its high index.

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