Identification of Cleavage Planes in Fully Networked Structures

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The cleavage of materials provides a process to create atomically smooth surfaces. To identify possible cleavage planes in materials, we start from the atomic bonding network of a three dimensional solid and systematically break bonds within the network. For each material in the Materials Project database with a primitive cell of up to 15 atoms, we break up to four bonds within solids that are fully networked and analyze the dimensionality of the resulting bonding network. Successful cleavage reduces the network dimensionality to two, i.e., a slab or monolayer. To characterize the likelihood of cleavage, we calculate the energy of adhesion and the relaxed surface energy of these slabs. Comparing these values to those of known substrates, we create a list of candidate cleavage planes and discuss the stability of these surfaces with respect to the number of broken bonds and coordination numbers. We predict 3423 cleavage planes across 1847 materials, identifying both novel substrate materials and several surfaces that meet the stability of a freestanding monolayer.