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Surface energy anisotropy for FCC metals: Functional forms YAN-JIUN CHEN, MIHIR KHADILKAR, JAMES P. SETHNA, LASSP, Cornell University — The energy of a crystalline surface depends on the angle of the surface normal with respect to the crystalline axes (i.e. the Miller index). We show that the surface energy as a function of angle is surprisingly easy to describe with a simplistic broken bond model including only a few parameters. In particular, this model is successful at capturing the cusps at high symmetry surfaces. We will use our fitted functional form as a characteristic continuum description of material surface energies for FCC metals. The anisotropy of these surface energies can then be utilized in the study of many material properties- equilibrium shapes (Wolff plots) of crystals and voids, fracture mechanics, cleavage and faceting. We calculate the surface energies using ab initio calculations and various interatomic potentials, providing a measure of the fitness of the potentials for studying physical systems with surfaces. Furthermore, we assemble systematic tables of these results, available to the community through the Knowledgebase of Interatomic Models (KIM, https://openkim.org/).

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