1125-70-1381 **Tim Krumwiede*** (krumwiede@math.utk.edu), 2704 Sood Rd Apt 9, Knoxville, TN 37921, and **Tim P Schulze**. *Surface Energy in Bond-Counting Models.* Preliminary report.

Continuum models in computational material science require the choice of a surface energy function, based on properties of the material of interest. I will show how to use atomistic stochastic bond-counting models and crystal geometry to inform this choice. We will examine some of the difficulties that arise in the comparison between these models due to differing types of truncation. New crystal geometry methods are required when considering materials with non-Bravais lattice structure, resulting in a multi-valued surface energy. I will present these methods in the context of the two-dimensional material graphene in a way that correctly predicts its equilibrium shape. (Received September 16, 2016)