Abstract: Crystalline organic solids are ubiquitous as either final products or as intermediates in the specialty chemical, pharmaceutical, and home & personal care industries. Virtually all small molecular weight drugs are isolated as crystalline materials, and over 90% of all pharmaceutical products are formulated in particulate, generally crystalline form. Normally, the properties of the crystalline solid (especially polymorph and crystal shape) have a major impact on the functionality of the product as well as the design and operation of the manufacturing process, and in most cases the two cannot considered separately. The current generation of process models for solution crystallization focus on the prediction of particle size distribution for populations of spherical particles. In this modeling environment the growth models are isotropic, and are incapable of predicting the shapes of faceted crystals. Crystal shape, however, is an important material characteristic and there is significant potential value for process models that are capable of simultaneous prediction of crystal size and shape. To be successful in a process simulation environment, shape prediction models must be fast (they will get called hundreds or even thousands of times during a process simulation) and yet faithful to the fundamental chemical physics and interactions governing the development and evolution of crystal shape. To predict crystal shape it is necessary to predict the relative growth rates of the faces which appear on the crystal surface. The rate determining step for the growth of most API crystal faces is surface integration kinetics of solute molecules. Based on this, we have succeeded in developing the first ever ab initio mechanistic model for predicting the relative growth rates of non-centrosymmetric organic molecules of realistic complexity. The key variables on which the model depends are (1) properties of the solid state, such as unit cell, space group, intermolecular potentials, charge distribution, etc, (2) properties of steps and kinks (kink rates that account for non-isotropic behavior, treatment of unstable edges, modified Boltzmann kink distribution), and (3) surface free energy at the crystal-solution interface. The model has been successfully applied to a selection of complex molecular crystals of interest in pharmaceutical and specialty chemical products.