Kinetic Wulff Construction for Twinned Particles

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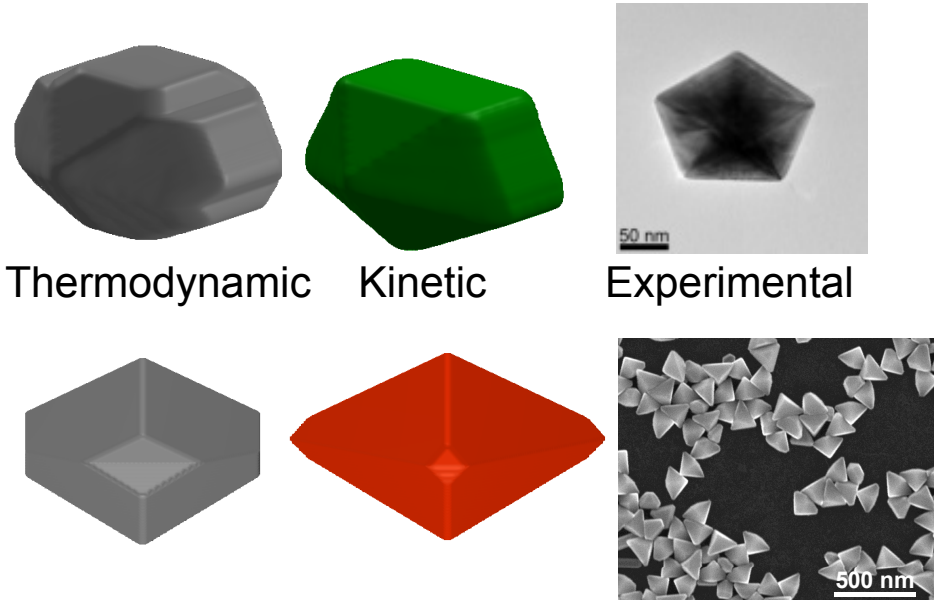
The **Marks** group developed a new theoretical approach describing the shape of particles grown in non-equilibrium reactions. Such particles could not be modeled previously, as they are not thermodynamic products. The kinetic Wulff model uses surface growth velocities instead of surface energies, and growth enhancement parameters are included, accounting for the easy nucleation at crystallographic defects and concave surfaces. This approach is able to predict the formation of a variety of common shapes left unexplained by thermodynamic modeling, such as sharp bipyramids and decahedra.



Thermodynamic and kinetic shapes for decahedral (top) and singly twinned (bottom) nanoparticles. Adjacent shapes were modelled with identical surface growth velocity, but kinetic enhancement was applied to obtain the green and red shapes. Nanoparticles pictures on the right were synthesized by the Mirkin group (IRG-3).

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