

Abstract Submitted
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Ab Initio Insights on the Shapes of Nanocrystals¹ ROMAN CHEPULSKYY, STEFANO CURTAROLO, Duke University — Catalytic, chemical, optical and electronic properties of nanocrystals are strongly influenced by their faceting. A variational approach based on quantum mechanical energies is introduced to evaluate stable and metastable shapes of nanocrystals. The method leads to a nanoscale equation of state, which is solved self-consistently. Using platinum as example, it is found that the surface energy dependence on the lattice parameter is the key factor controlling the equilibrium stability of the crystal shapes. The energies of different surfaces versus lattice parameter are calculated from first principles in high-throughput fashion. Considering several crystal shapes and using Wulff's construction, the transitions between stable and metastable shapes are predicted below 3 nm in diameter. Our variational approach explains experimental results and establishes a direction to search for better catalysts.

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