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Equilibrium and metastable shapes of platinum nanoparticles from first principles[1] ROMAN CHEPULSKYY, Duke University, STEFANO CURTAROLO, Duke University and Weizmann Institute of Science — An approach for prediction of stable and metastable shapes of nanoparticles as function of their size is developed. It is based on first principles calculation of high-index surface-energies and nanoparticle surface-tension excess free energies without phenomenological approximations. The approach is applied in the case of platinum nanoparticles as being one of the most used catalysts. The theoretical predictions are verified by comparison with direct first principles calculations for small clusters.

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