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Tangential Ligand-Induced Strain in Icosahedral Au13 LEEOR KRONIK, OLGA GULIAMOV, Weizmann Institute of Science, ANATOLY FRENKEL, Yeshiva University, LAURENT MENARD, RALPH NUZZO, University of Illinois — A quantitative comparison of first principles calculations with extended x-ray absorption fine structure and transmission electron microscopy measurements provides strong evidence that Au_{13} nanocrystals are stabilized in a slightly distorted icosahedral structure by on-top phosphine ligands and a combination of on-top and bridging thiol ligands. Importantly, the ligands change the icosahedral strain (i.e. the radial- tangential bond length ratio) significantly, with the tangential bonds within the Au core exhibiting much more disorder than the radial ones.

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