ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ

ΤΜΗΜΑ ΦΥΣΙΚΗΣ

ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

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17:00 -18:00

3rd Floor Seminar Room

"Equilibrium shape of nanoparticles from first principles"

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Abstract

Metal nanoparticles in heterogeneous or homogeneous suspensions have important technological applications due to their unique catalytic and optical properties. For example, oxide-supported Au nanoparticles is the best-known catalyst for room-temperature oxidation of poisonous CO to CO2. The equilibrium shape of nanoparticles can be calculated from first-principles atomistic simulations with the use of the Wulff-Kaishew theorem and its generalizations. One first calculates the surface tension of various (hkl) surfaces and then finds the shape that gives minimum surface energy for given number of atoms.
In this talk, we discuss recent applications of this methodology to a variety of materials including Ru particles in ammonia-synthesis catalysts, Si quantum dots in amorphous SiO2, diamond nanocrystals in amorphous C, and, most recently, Au nanoparticles in both inert and reactive environment. We compare our findings to experimental observations and discuss potential applications.