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In Situ Characterization of Nanostructures Using Rayleigh Scattering¹ BISWAJIT SANTRA, MIKHAIL N. SHNEIDER, ROBERTO CAR, Princeton University, Princeton, USA — Controlling selective growth of nanotubes has posed a considerable challenge over the last two decades. A crucial step to overcoming such hurdle is to gain detailed knowledge of the early stage of nanomaterial syntheses for which *in situ* measurements are required. Laser-based probes, such as Rayleigh scattering (RS), can potentially characterize the shape and size of nanoparticles *in situ*. The intensity of RS in a gas mixed with nanoparticles is proportional to the polarizabilities of the constituent particles, therefore, theoretical spectroscopy can complement such measurements. Here, we employed time-dependent density functional theory to compute the frequency-dependent polarizabilities of various nanostructures and predicted the corresponding RS intensity and depolarization. We found that with increasing length and asymmetry of the nanostructures the longitudinal polarizability exhibited characteristic resonances leading to measurable signatures in the RS intensity and depolarization. Also by considering gas-particle mixtures at estimated experimental conditions for nanoparticle synthesis on the periphery of an arch, we predict that *in situ* characterization of a few nanometer long particles with concentration as low as one particle per million is feasible using RS.

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