Quantum plasmonics of stretched nanorods

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The capability to control the optical response of metallic nanoparticles is a key factor for the diverse application potential of nanoplasmonics. In systems with increasingly miniaturized features, the response is affected by emerging quantum phenomena. A prototypical system is the metallic nanoparticle dimer in which electron tunneling strongly affects the plasmonic response at subnanometer particle separations [1, 2].

In this work, we realize the dimer system as the end result from the stretching of a metallic nanorod. Starting from a perfect nanorod, we track the evolution of the plasmon modes with first-principles time-dependent density-functional theory calculations. The stretching process is characterized by the formation of a narrowing atomic contact between the nanorod ends until the rod is eventually split into two smaller nanorods. In between the limiting cases of a single nanorod and a nanorod dimer, the plasmonic response of the system shows novel quantum features [3]. These features and their origin are discussed in detail in the presentation.