Numerical studies on nearly touching plasmonic nanoparticle dimers

Xudong Cui and Daniel Erni

General and Theoretical Electrical Engineering (ATE), Faculty of Engineering,
University of Duisburg-Essen, D-47048, Duisburg, Germany

Nearly touching metallic nanoparticle dimers have attracted intense interest in current plasmonic research, since huge field enhancements are typically observed in the gap region of the two particles, especially in the potential contact region. A huge field enhancement is beneficial to the creation of so-called 'hot-spots', which are crucial to Surface Enhanced Raman Scattering (SERS), sensing, single molecule detection, as well as to the emergent realm of non-linear plasmonics. With the development of nanofabrication and experimental techniques, small gap size in the order of ~1nm becomes practically feasible. Although nanoparticle dimers have been intensively investigated, simulations for nearly touching dimers are barely seen in current literature. Nevertheless, numerical simulations are mandatory to better understand recent experimental results, not to mention the underlying physical mechanisms. The major challenges for such kind of numerical analysis are the following: for instance, to correctly address the field between such a tiny gap extremely fine meshes are needed, which inevitably results in large matrices and long computation time. Meanwhile, calculations become unstable and convergence is degraded due to the extremely small mesh cells. In the presented work, the Multiple Multipole Program (MMP), a frequency-domain based boundary element method is used to investigate the optical properties of the plasmonic dimer. The overall simulations are carried out within moderate computation time while showing fast convergence. Two regions are considered in the calculation: (1) a gap distance between 2 nm and 10 nm, where no charge transfer occurs between the two particles; and (2) the gap distance becomes less than 1 nm where electron tunneling is supposed to be present. Our results show a good agreement with experimental findings. Finally, a finite element code is employed for comparison reasons.