IT Services

Case Study

BlueBEAR provides a substantial computing resource that properly supports the research work of research staff and students at Birmingham. It provides a cost effective facility that optimises the effectiveness of research and ensures the University continues to be a world-class academic learning and research environment.

Theoretical Studies of the Optical Properties of Gold and Palladium Nanoparticles

Challenges

To identify the different geometrical features of metallic nanoparticles which contribute to their varied optical properties.

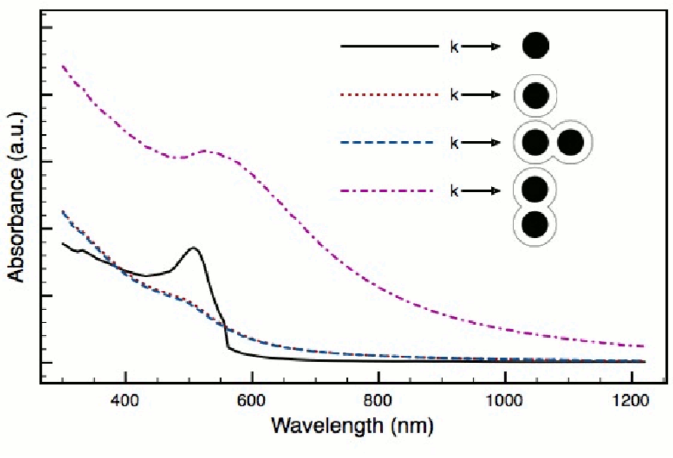
Background

The excitation of surface-plasmons by light on planar surfaces is called surface-plasmon resonance (SPR), or localised surface plasmon resonance (LSPR) for metal clusters in the nanometre size range. Nanoplasmonics has received considerable attention in recent times due to technological advances which now allow us to manipulate and structurally characterise clusters on the nanometre scale, and the resulting important applications of these features e.g. sensors. The optical properties of nanoparticles are size and shape dependent, allowing for tunability; in the case of heterogeneous nanoclusters composition also contributes. Nanorod shapes are of particular current interest due to their display of two axis-dependent SPRs [2].

Results

Research focuses on calculations using the discrete dipole approximation (DDA) to model the interaction of light with homo- and hetero-geneous metallic nanoparticles of varied shapes and sizes. Typically, calculations consist of over 100,000 dipolar points (N), and with 3N linear equations to be solved the process can become very computationally expensive. The BEAR cluster allows high-class computational facilities to perform these calculations. From our results we can then draw up simulated UV-Vis absorption spectra for these nanoparticles, and compare them with experimental data to identify distinct contributing features, thus aiding the experimentalists work towards nanoparticles which are very wavelength specific in their responses [3].

[1] F. Baletto and R. Ferrando. Rev. Mod. Phys., 77:371–423, 2005.
[2] E. S. Kooij and B. Poelsema. Phys. Chem. Chem. Phys., 8:3349–3357, 2006.
[3] A. Logsdail, N. J. Cookson, S. L. Horswell, Z. W. Wang, Z. Y. Li and R. L. Johnston, ACS Nano, submitted, 2010.



DDSCAT calculations for isolated Au and Au(core)Pd(shell) spheres compared to Au(core)Pd (shell) particles oriented with conjoining axis parallel and perpendicular to light (k). Au and Pd are represented in the schematics by black and white, respectively.

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Product Used
DDSCAT v7.0

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