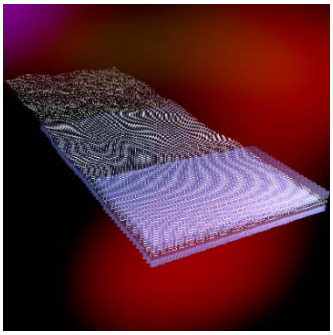
Center for Nanostructured Graphene - Highlights in 2017

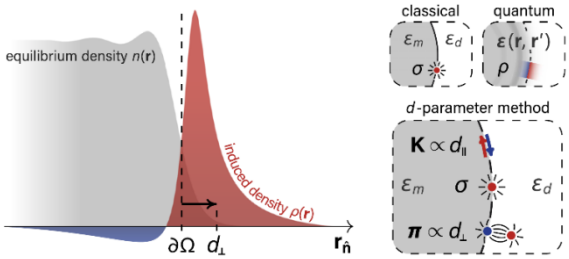
Suppression of intrinsic roughness in encapsulated graphene



When a two-dimensional material like graphene is suspended in free space, it is not perfectly flat. Instead, the surface becomes rippled like the surface of a pond on a windy day. This unavoidable roughness is caused by the non-zero temperature of the material, and leads to scattering of charge carriers that can reduce the performance of electronic devices made from graphene. Thomsen et al. showed that when a layer of graphene is sandwiched between layers of hexagonal boron nitride this roughness is greatly reduced. While this might be expected intuitively, what was not expected was just how flat the graphene can be. Using electron diffraction-based measurements in the transmission electron microscope, they showed that the roughness of such a sandwiched graphene layer is very close to the roughness of individual layers in a naturally occurring layered crystal like graphite, only a few tens of picometers (1 pm = 10^{-12} m) – the lowest roughness ever measured for a two-dimensional material. Simulations show that the thermal vibrations that are responsible for roughness become localised in the hexagonal boron nitride, leading to smoother graphene. What this means is that we can now artificially assemble two-dimensional materials into so-called van der Waals heterostructures with near perfect interfaces.

Thomsen, J. D., Gunst, T., Gregersen, S. S., Gammelgaard, L., Jessen, B. S., Mackenzie, D. M. A., Watanabe, K., Taniguchi, T., Bøggild, P. and Booth, T. J. (2017) Suppression of intrinsic roughness in encapsulated graphene, Physical Review B 96 (1), 014101, DOI: 10.1103/PhysRevB.96.014101 (Editor's recommendation)

Quantum corrections in nanoplasmonics: Shape, scale, and material

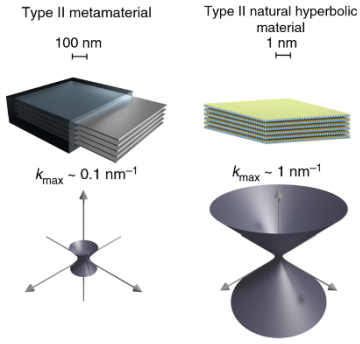


Since 1980's it has been well-known that a classical theory fails to account the plasmonic properties if the plasmon wave-length, or the geometric length-scales are below 5-10 nm. Experiments show that the resonance frequency for noble metal nanoparticles (e.g. Ag) shifts towards higher energies ("blue shift") while nanoparticles made of simple metals (e.g. Na) show an opposite trend ("red shift"), when compared to the size-dependence predicted by the classical theory. Two complementary theoretical approaches have been used to explain these observations: *ab inito* computations, or semiclassical models. *Ab initio* theories, usually based on the time-dependent density-functional theory (TDDFT) yield useful insight for the plasmonic frequencies for simple metals, but are computationally limited to nanoparticles consisting at most a few thousand atoms.

Semiclassical models, and in particular the hydrodynamical model, agree with experiments for noble metals, even in macroscopic geometries. However, they predict a wrong shift for simple metals. T. Christensen and co-workers have formulated an intermediate approach, which combines the precision of *ab initio* computations with the intuitive interpretation and computational advantages of the semiclassical approach. This has been achieved by introducing a set of surface-dependent response parameters, thereby generalizing the well-known Feibelman d-parameters. These parameters complement the conventional macroscopic permittivity in nanoscale geometries, and give rise to quantum mechanical shifts and broadening of plasmonic resonances, in accordance with experimental trends.

Christensen, T., Yan, W., Jauho, A.-P., Soljačić, M. and Mortensen, N. A. (2017) Quantum corrections in nanoplasmonics: Shape, scale, and material, Physical Review Letters 118 (15), 157402, DOI: 10.1103/PhysRevLett.118.157402 (WoS highly-cited article)

Layered van der Waals crystals with hyperbolic light dispersion



Electromagnetic metamaterials are artificially created, structured materials with unique optical properties. Hyperbolic metamaterials (HMM) have dielectric properties (ε>0) in one direction and metallic properties (ε < 0) in two orthogonal directions. The solution of Maxwell's equation then yields waves with hyperbolic rather than spherical/ellipsoidal isofrequency surfaces in reciprocal space. In principle, a hyperbolic dispersion implies divergent photonic density of states leading to high Purcell effects allowing for radiative decay engineering useful for applications such as single-photon light sources. However, in practice the hyperbolic isofrequency surface extends only up to wavevectors of size 1/a, where a is the periodicity of the structure. For conventional HMM, the periodicity is too large to yield a sufficient number of hyperbolic light modes (a is on the order of 100 nanometers). M. N. Gjerding and coworkers have demonstrated, using atomic-scale computer simulations that the broad class of layered transition metal dichalcogenides (TMDs) are naturally hyperbolic. Compared to artificially structured metamaterials, the absence of internal structure reduces (a is around 1 nanometer) greatly increases the number of hyperbolic modes, and significantly improves their photonic properties. The authors further show that the hyperbolic dispersion can be controlled by combining different two-dimensional crystals into van der Waals heterostructures opening up radically new opportunities for controlling light-matter interactions.

Gjerding, M. N., Petersen, R., Pedersen, T. G., Mortensen, N. A. and Thygesen, K. S. (2017) Layered van der waals crystals with hyperbolic light dispersion, Nature Communications 8 (1), 320, DOI: 10.1038/s41467-017-00412-y