

resonant wavelength, providing a spectral selectivity not observed in unconfined graphene. Similarly, when a current is applied to unconfined graphene, it

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heats up and emits a featureless thermal spectrum, whereas the graphene in the optical cavity displays a strong emission peak at the resonant wavelength.

Bio Focus

Weakly charged cationic nanoparticles unzip DNA

Inderstanding the interaction between charged nanoparticles and double-stranded DNA has important implications for drug delivery schemes and DNA-templated metallization, in addition to other possible applications. While attempting to package DNA onto nanoparticles as a means of gene delivery into cells, Anatoli V. Melechko of North Carolina State University (NCSU), Timothy E. McKnight of Oak Ridge National Laboratory, and their colleagues discovered something completely unexpected. Some of the nanoparticles clumped together, and in the process pulled the double-stranded DNA apart, at least partially.

"This could be a new type of machinery that can be used for separating DNA into single strands," Melechko said, admitting that a lot more work will need to be done to understand and control the phenomenon.

In nature, negatively charged DNA wraps around protein cylinders with a positive charge of +220 to form a com-

plex known as chromatin. A high positive charge on a protein or a nanoparticle causes DNA to bend and undergo compaction. Much work has been done with functionalized nanoparticles in this regime. Some research has been done with weakly positive charged nanoparticles, which typically have no effect on the conformation of DNA. In choosing gold nanoparticles (AuNPs) functionalized with thiolated alkane ligands bearing primary amines with a charge of +6, Melechko and his colleagues explored the lesser-known transition charge region between the weak and the strong regimes.

As reported in the August 16 issue of *Advanced Materials* (DOI: 10.1002/ adma.201104891; p. 4261), gel electrophoresis experiments with the AuNP-DNA showed a "mystery band in a gel an extra line [close to the 1000 base pair marker] that created the main puzzle for us," Melechko said. Though prior work by others might signify that this mystery line was the result of DNA compaction affecting gel mobility, Melechko and coworkers hypothesized that some denaturing—or unzipping—of the two-stranded DNA was occurring. UV spectroscopy The researchers also found that confined graphene exhibited unusual electrical behavior. At low voltages the cavity inhibits the emission of the low energy thermal radiation with wavelengths longer than resonance, and the current therefore saturates. As the voltage is increased, this threshold for light emission is passed and the device resistance drops accordingly.

Graphene is an ideal material for this type of device because of its twodimensional nature, which allows it to extend for micrometers across the center of the cavity, and easily tunable electrical properties. The degree of spectral selectivity provided by the optical confinement suggests a useful application in photodetection, while its influence on electrical transport could be exploited in nanoelectronic devices.

Tobias Lockwood

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To better understand the phenomenon, co-researcher Yaroslava Yingling of NCSU ran molecular dynamics simulations involving single AuNPs with six charged ligands (AuNP-6NH₃⁺), and compared them with other molecular dynamics simulations involving three of the AuNP-6NH₃⁺ units. The singleparticle simulations showed binding of the ligands to both the minor and major grooves of DNA, but little structural alteration in the double helix. Basically, the DNA just sticks to a single nanoparticle. But in the three-particle simulations, the nanoparticles bunch together. "You have hydrophobic groups that want to hide between themselves, and polar groups that grab on to DNA," Melechko said. "When they do this clumping and still hold on to DNA, they can rip it apart."

The researchers said that "particles acting in concert can produce effects not possible with single particles." A video of the molecular dynamics simulation can be viewed at http://youtu.be/9M-58niEOpU.

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