Developing better nano-electronics by understanding nonadiabatic effects

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"Basically," Michele Lazzeri tells *PhysOrg.com*, "the Born-Oppenheimer adiabatic approximation tells us how atoms are vibrating." This adiabatic effect is used to describe phonons, which are modes of vibration that have been quantized. "It's basic textbook stuff in solid state physics," Lazzeri continues, "but sometimes the Born-Oppenheimer adiabatic approximation fails."

This failure is known as nonadiabatic effects. However, even though the existence of such has been speculated about since the 1960s, measuring – and understanding – how nonadiabatic effects affect solids has been difficult, especially in terms of distinguishing them in new materials such as graphene and carbon nanotubes. (It is important to note that graphene and nanotubes hold a great deal of interest in nanotechnologies, they are considered as potential components for future nano-electronic-devices.)

Lazzeri, along with A. Marco Saitta, Matteo Calandra and Francesco Mauri, all at IMPMC at the University of Paris 6, have created a theoretical framework for explaining nonadiabatic effects, and their differences from adiabatic effects. Their work has been published in *Physical Review Letters*: "Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained."

"Our work is really a scientific curiosity," Lazzeri explains. "Efforts have been made to use Raman spectroscopy to detect and measure these nonadiabatic effects in metals." Nonadiabatic effects can be used to

explain certain properties seen due to Raman scattering, including linewidths and shifts. “It’s really about understanding basic principles in quantum mechanics.”

What prompted the present work was actually work that the University of Paris team had done earlier, looking for nonadiabatic effects in graphene. “It turns out that graphene dependence to phonon frequency on doping, or adding electrons, is due to nonadiabatic effects.” However, the difference between the adiabatic and the nonadiabatic was not very pronounced in graphene, making it difficult to measure. So the Lazzeri and his peers wondered what would happen if they used layered metals that were truly three dimensional, rather than closer to two dimensional, as graphene is.

“We realized that when you have layered material, like the intercalated graphite and the MgB_2 [magnesium diboride] used in the experiments we studied, you can do Raman scattering to excite the phonons to where the Born-Oppenheimer approximation fails,” Lazzeri says. This is done, he explains, by probing with a laser direction that is perpendicular to the layers.

“We found that the difference between the adiabatic and the nonadiabatic effects were huge in these cases,” he continues. “The difference is much more spectacular in the graphite than in the graphene we studied before.”

Lazzeri hopes that the information and first principles that the team articulates can be applied going forward to other new materials to be used in future nano-electronic devices. “It does have a technology application,” he insists.

“The study of vibrations is not only interesting from a purely scientific point of view,” he continues. “As a matter of fact, vibrations provide us

with one of the most direct access to the properties of matter at the microscopic level."