Study sheds light on—and through—2-D materials

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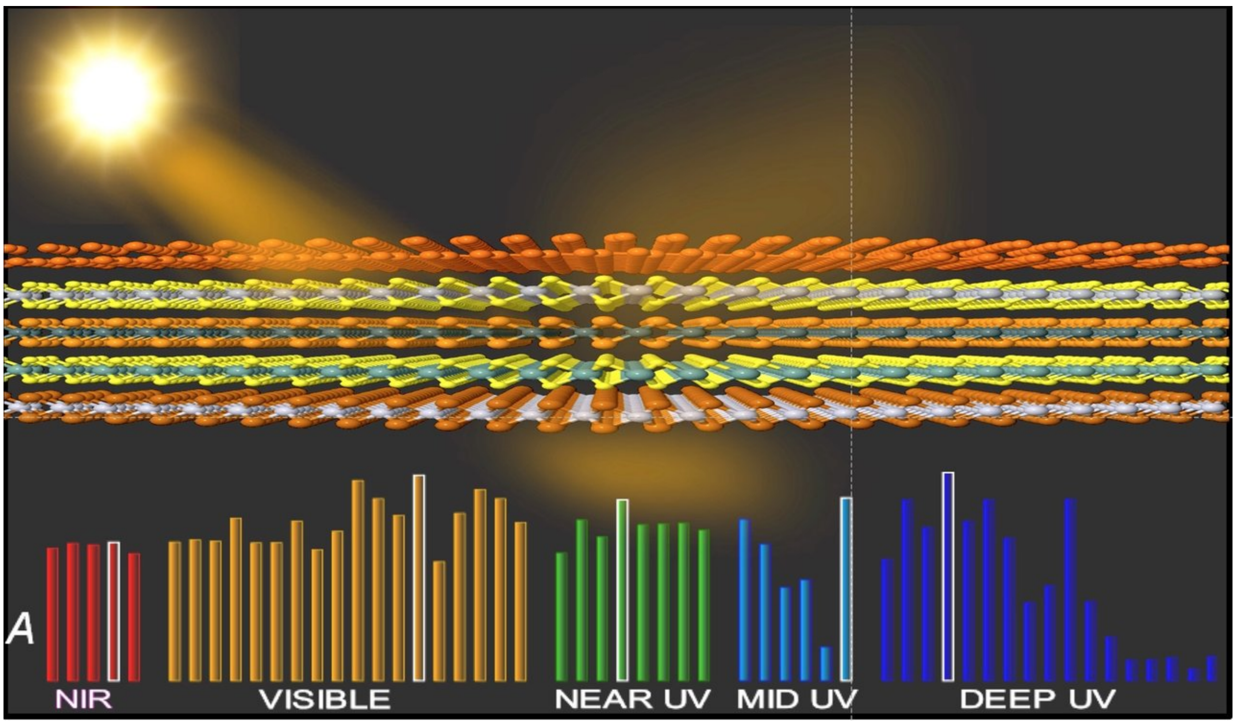

Rice University researchers modeled two-dimensional materials to quantify how they react to light. They calculated how the atom-thick materials in single or stacked layers would transmit, absorb and reflect light. The graphs above measure the maximum absorbance of several of the 55 materials tested. Credit: Yakobson Research Group/Rice University

The ability of metallic or semiconducting materials to absorb, reflect and act upon light is of primary importance to scientists developing optoelectronics—electronic devices that interact with light to perform tasks. Rice University scientists have now produced a method to determine the properties of atom-thin materials that promise to refine the modulation and manipulation of light.

Two-dimensional materials have been a hot research topic since graphene, a flat lattice of carbon atoms, was identified in 2001. Since then, scientists have raced to develop, either in theory or in the lab, novel 2-D materials with a range of optical, electronic and physical properties.

Until now, they have lacked a comprehensive guide to the optical properties those materials offer as ultrathin reflectors, transmitters or absorbers.

The Rice lab of materials theorist Boris Yakobson took up the challenge. Yakobson and his co-authors, graduate student and lead author Sunny Gupta, postdoctoral researcher Sharmila Shirodkar and research scientist Alex Kutana, used state-of-the-art theoretical methods to compute the maximum optical properties of 55 2-D materials.

"The important thing now that we understand the protocol is that we can use it to analyze any 2-D material," Gupta said. "This is a big computational effort, but now it's possible to evaluate any material at a deeper quantitative level."

Their work, which appears this month in the American Chemical Society journal *ACS Nano*, details the monolayers' transmittance, absorbance and reflectance, properties they collectively dubbed TAR. At the nanoscale, light can interact with materials in unique ways, prompting electron-photon interactions or triggering plasmons that absorb light at one frequency and emit it in another.

Manipulating 2-D materials lets researchers design ever smaller devices like sensors or light-driven circuits. But first it helps to know how sensitive a material is to a particular wavelength of light, from infrared to visible colors to ultraviolet.

"Generally, the common wisdom is that 2-D materials are so thin that they should appear to be essentially transparent, with negligible reflection and absorption," Yakobson said. "Surprisingly, we found that each material has an expressive optical signature, with a large portion of light of a particular color (wavelength) being absorbed or reflected."

The co-authors anticipate photodetecting and modulating devices and polarizing filters are possible applications for 2-D materials that have directionally dependent optical properties. "Multilayer coatings could provide good protection from radiation or light, like from lasers," Shirodkar said. "In the latter case, heterostructured (multilayered) films—coatings of complementary materials—may be needed. Greater intensities of light could produce nonlinear effects, and accounting for those will certainly require further research."

The researchers modeled 2-D stacks as well as single layers. "Stacks can broaden the spectral range or bring about new functionality, like polarizers," Kutana said. "We can think about using stacked heterostructure patterns to store information or even for cryptography."

Among their results, the researchers verified that stacks of graphene and borophene are highly reflective of mid-infrared light. Their most striking discovery was that a material made of more than 100 single-atom layers of boron—which would still be only about 40 nanometers thick—would reflect more than 99 percent of light from the infrared to ultraviolet, outperforming doped graphene and bulk silver.

There's a side benefit that fits with Yakobson's artistic sensibility as well. "Now that we know the optical properties of all these materials—the colors they reflect and transmit when hit with light—we can think about making Tiffany-style stained-glass windows on the nanoscale," he said. "That would be fantastic!"

More information: Sunny Gupta et al, In Pursuit of 2D Materials for Maximum Optical Response, *ACS Nano* (2018). DOI: 10.1021/acsnano.8b03754

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