Researchers develop new model to predict the optical properties of nanostructures

March 24 2011

University of British Columbia chemists have developed a new model to predict the optical properties of non-conducting ultra-fine particles.

The finding could help inform the design of tailored nano-structures, and be of utility in a wide range of fields, including the remote sensing of atmospheric pollutants and the study of cosmic dust formation.

Aerosols and nano-particles play a key role in atmospheric processes as industrial pollutants, in interstellar chemistry and in drug delivery systems, and have become an increasingly important area of research. They are often complex particles made up of simpler building blocks.

Now research published this week by UBC chemists indicates that the optical properties of more complex non-conducting nano-structures can be predicted based on an understanding of the simple nano-objects that make them up. Those optical properties in turn give researchers and engineers an understanding of the particle's structure.

"Engineering complex nano-structures with particular infrared responses typically involves hugely complex calculations and is a bit hit and miss," says Thomas Preston, a researcher with the UBC Department of Chemistry.

"Our solution is a relatively simple model that could help guide us in more efficiently engineering nano-materials with the properties we want, and help us understand the properties of these small particles that play an

important role in so many processes."

The findings were published in the Proceedings of the National Academy of Sciences.

"For example, the properties of a more complex particle made up of a cavity and a core structure can be understood as a hybrid of the individual pieces that make it up," says UBC Professor Ruth Signorell, an expert on the characterization of molecular nano-particles and aerosols and co-author of the study.

The experiment also tested the model against CO2 aerosols with a cubic shape, which play a role in cloud formation on Mars.

More information: Read the paper in the *Proceedings of the National Academy of Sciences*: www.pnas.org/content/early/201 … /1100170108.abstract

Provided by University of British Columbia