Jumping Crystals: Terahertz Phonons Dictate Macroscopic Mechanical Dynamics in Organic Materials

Speaker

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Over the past two decades, terahertz time-domain spectroscopy has become a valuable technique for the characterization of solid samples, primarily due to its sensitivity to bulk molecular packing arrangements. This has made terahertz spectroscopy a powerful tool for studying crystalline polymorphism, and has also aided in structural determination work. This is because of the extreme and direct sensitivity of terahertz phonons to weak, often non-covalent, interactions in the condensed phase. Additionally, in recent years, the role that specific terahertz vibrations play in a number of important physical phenomena has become increasingly apparent, with numerous studies highlighting how terahertz motions are directly responsible for the proper functioning of materials, ranging from enzymatic catalysis to solid-state phase transformations. In the latter case, there have been several examples where terahertz phonons have been shown to map out the reaction pathways associated with structural changes, often induced by external perturbations such as temperature or pressure. Recently, a class of compounds that exhibit macroscopic changes in structure, i.e., the shape and size of micro- and millimeter-sized crystals, have been discovered. Many of these materials exhibit bulk dynamics, for example crystals that literally 'jump' when undergoing a phase transformation, which has led to suggested uses for such materials in applications such as mechanical actuators. In this work, we probe the reaction mechanisms in these materials using terahertz spectroscopies, including both terahertz time-domain spectroscopy and low-frequency Raman spectroscopy. Here, specific terahertz motions are identified that are responsible for such phenomena, enabling a direct 1-to-1 mapping of critical processes to a low-frequency vibrational resonance. This is applied to a variety of crystals, including ferroelectrics and porous materials. Overall, this work highlights the powerful role that low-frequency vibrational spectroscopy can play in characterizing and understanding the structures and properties of advanced organic materials.

Michael Ruggiero *is Associate Professor of Chemistry and Chemical Engineering at the University of Rochester. He received his BS from SUNY Geneseo and PhD in chemistry from Syracuse University, and was an EPSRC postdoctoral fellow at the University of Cambridge in the Department of Chemical Engineering, followed by spending five years as an Assistant and Associate Professor at the University of Vermont. His research involves characterizing and leveraging intermolecular interactions in the condensed phase to understand bulk material function. While the applications of his research are broad – the core of his research program is centered on vibrational spectroscopy (in particular, low-frequency vibrational spectroscopy), crystallography, and ab initio simulations. He collaborates widely, contributes to the development of the CRYSTAL software package, has published over 60 peer-reviewed articles and he was previously a Topic Editor for Crystal Growth & Design and currently sits on the ACS Society Committee on Publications, which oversees the entire ACS publishing portfolio. He has been awarded over $3 million in external funds, including an NSF CAREER award, and is the recipient of a number of awards, most recently being included in the annual Forbes 30 Under 30 list (2019) and winning the Young Scientist Award by the International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz 2019).*

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