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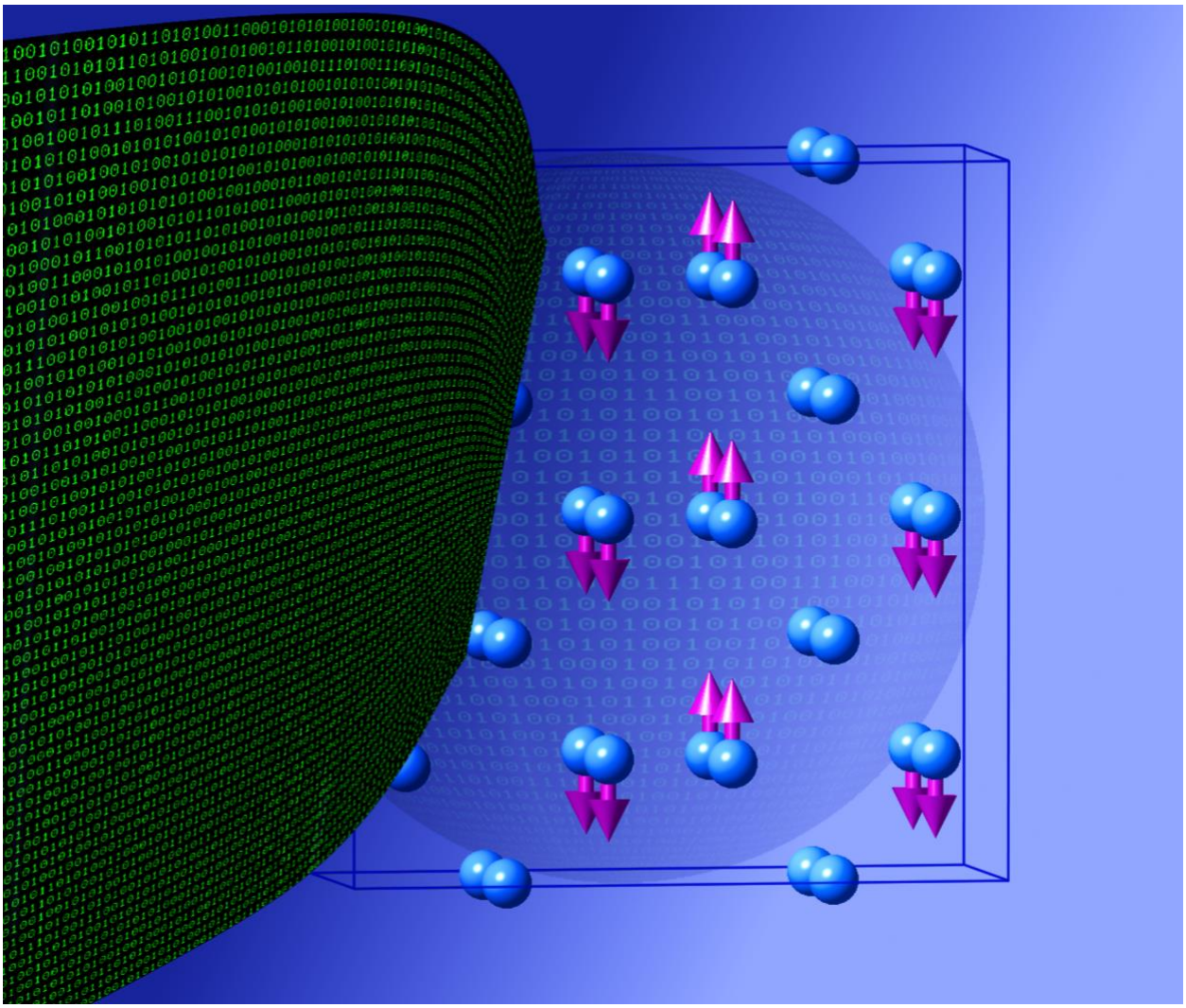
Natural Descriptors for Materials Dynamics

A new framework aims to help researchers understand, model, and tailor the non-linear, dynamical properties of materials.



The massive amount of data from molecular dynamics simulations of a material can be daunting. The new framework extracts the key collective atomic motion, paving the way to deeper understanding of materials and enabling better control of functionality.

The Science

Work in the Theoretical Division has introduced an advanced method to describe the movement of atoms in a material at finite temperatures that takes into account the atoms' collective movement. Rather than describing the movement in terms of generic static descriptors, which fail to give an intuitively accessible picture at the temperature of the material, the method relies on extracting the natural descriptors specific to the material at that temperature.

The Impact

The new framework provides a natural set of dynamics descriptors that stands to dramatically advance our understanding of how atoms collectively move. The descriptors provide the missing link between atomistic simulations and material behavior at different temperatures. From scientists designing new materials for specific functionality to researchers studying shock wave propagation, the descriptors represent a powerful addition to their toolbox.

Summary

Materials are increasingly studied with computer simulations. The data from the simulations allow the observation of how the behavior of the material differs with changes in pressure and temperature. But connecting the material behavior with how the atoms move has been challenging, because their movement becomes intertwined when described in traditional terms such as lattice vibration modes. The advance in the new framework comes from using the data itself to extract a measure of the intertwined movement, and then constructing a new set of modes that are no longer intertwined. To demonstrate the power of the new framework, the application to structural phase transformations shows that such transformations are described by just one single mode. This type of intuitive insight makes the increasing data flow amenable to human understanding.

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Publication

Sven P. Rudin, Generalization of soft phonon modes. Physical Review B **97**, 134114 (2018).

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https://journals.aps.org/prb/abstract/10.1103/PhysRevB.97.134114