COMMENTARY

Energy conversion materials need phonons

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Phonons, as bosonic particles unaffected by the Pauli exclusion principle or the Fermi level, are fundamental to understanding the physical properties of solid materials. Their interactions with electrons and the crystal lattices significantly influence transport phenomena, such as electrical conductivity, mobility, and magneto-transport processes. When an external electric field is applied to an electron within a solid, the electron interacts with lattice ions, causing distortions in the lattice. These distortions propagate as phonons, transferring the electron's energy and momentum, thus facilitating electron transport. By controlling phonons and their interactions with lattices and electrons, we can deepen our understanding of solid materials and enhance their applications in energy conservation.

ELECTRON-PHONON INTERACTION AND PHYSICAL PROPERTIES

Electron-phonon interactions primarily manifest through electron scattering processes. When an electron collides with a phonon, it transfers part of its energy and momentum to the lattice, increasing the amplitude of the lattice wave and raising its quantized energy level, thereby emitting a phonon. Conversely, if the lattice wave of a normal mode reduces its quantized energy level and transfers energy and momentum to the electron during the collision, the electron absorbs a phonon. This process of phonon emission and absorption is critical for electron transport. In some high-temperature superconductors, electron-phonon coupling leads to the formation of electron pairs, facilitating superconductivity.[1] Specifically, *p*-wave superconductivity can occur when electron-phonon coupling is localized in *q*-space. In certain topological semimetals, acoustic modes dominate scattering at low temperatures, while both acoustic and low-frequency optical modes contribute to scattering at higher temperatures—a key factor in low-temperature anomalous resistivity. Like electrons, phonons can also be described in topological terms, giving rise to topological phonons (TPs). These TPs can excite surface or edge states protected by nontrivial topology, enabling the directional transport of energy and signals along specific paths that are robust against scattering and interference.

CATALYSIS TALKS WITH PHONONS

As a medium for energy exchange between materials and their external environment, phonons play a vital role in catalysis. Phonon-based catalysis can maintain materials at low temperatures while utilizing the vibrations of selectively excited phonons to create the high-temperature conditions needed for reactions. This process alters the diffusivity of ions within the material, promoting ion diffusion, accelerating charge transfer, and improving conductivity. As a result, it is expected to mitigate the harsh high-temperature conditions typically required in fuel cells, thereby extending their operational lifespan.

In photothermal catalysis, the collective oscillation of surface electrons in metal nanoparticles generates high-energy "hot" carriers. These carriers possess enough energy to escape the plasma and trigger surface chemical reactions. Carriers that lack sufficient energy for surface charge transfer are instead converted into metal lattice phonons through electron-lattice collisions. This raises the temperature of the metal lattice, which then propagates to the surrounding surface through phonon-phonon scattering. When the lattice vibration of the catalyst

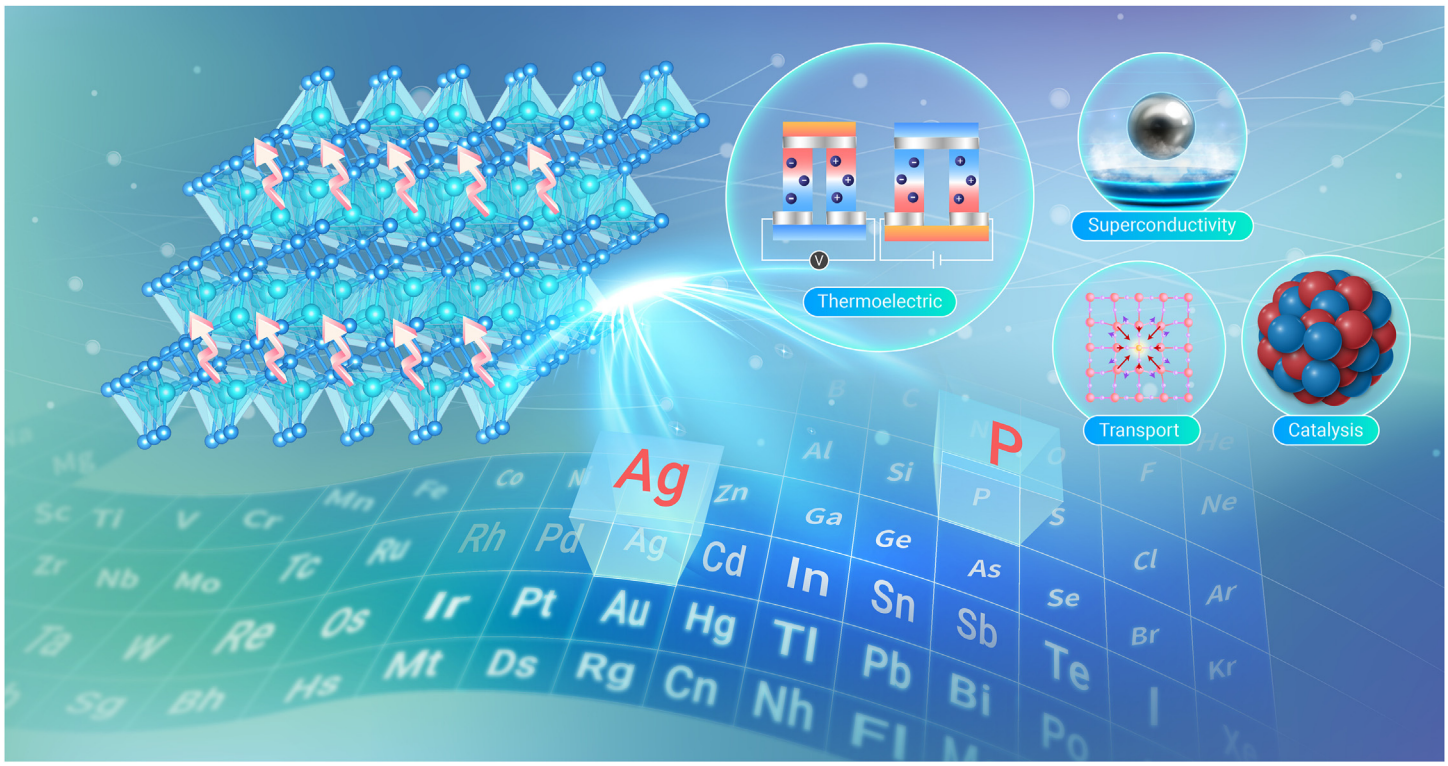

Figure 1. Application of the TP database in the search for energy materials

resonates with molecular vibrations, energy is transferred directionally along the reaction path. The resonance intensifies the corresponding vibrational modes until the molecular bond breaks, lowering the Gibbs activation energy of the reaction.[2]

In semiconductor materials, when incident light has energy equal to or greater than the band-gap energy, electrons quickly transition to lower energy states, releasing energy in the form of lattice phonons. This conversion of photons to phonons increases the temperature of the semiconductor, further enhancing catalytic performance and quantum efficiency. Phonons can also serve as a powerful driving force for reactions by coordinating the interaction between photons and phonons, promoting bond dissociation, and improving the adsorption/desorption of reactants and intermediates.

TP MATERIALS: EXCEEDING EXPECTATIONS

Unlike electrons, which can be detected through various transport experiments and spectroscopy with ultra-high energy resolution, phonons are largely insensitive to external electric or magnetic fields. Their detection is limited to a few large-scale scientific instruments, such as inelastic X-ray scattering, neutron scattering techniques, and electron energy-loss spectroscopy. Additionally, calculating phonon properties is time consuming and labor intensive, which has led to a scarcity of newly discovered TP states and ideal TP materials.[3] These limitations have significantly hindered the development of phonon-based catalysis. Key challenges include identifying which phonon vibration modes dominate ion diffusion, understanding how phonons transfer energy to drive catalytic reactions, regulating electron-phonon interactions, reducing reaction barriers, enhancing phonon catalysis efficiency, and designing stable, efficient phonon catalysts.

To tackle these challenges, Xu et al. developed a catalog of TP bands for over 10,000 three-dimensional crystalline materials using spinless topological quantum chemistry and high-throughput computation.[4] This phonon database offers a comprehensive topological classification of phonon bands for each material, including irreducible representations, compatibility relations, and topological indices (Figure 1). The resource is freely accessible at https://www.topologicalquantumchemistry.fr/topophonons/ and features a flexible search engine designed to accelerate TP materials development. Interestingly, nontrivial band topologies are found to be widespread in phonon systems, with approximately 52.98% of the materials exhibiting various forms of topology in surface phonon dispersion, including strong or fragile topologies, obstructed atomic band representation (OABR), orbital-selected OABR (OOABR), and symmetry-enforced band nodes. This authors applied strict filtering criteria based on crystal structure stability and energy resolution, identifying ideal phonon materials with strong (187, 1.63%), OABR (1430, 12.43%), and OOABR (623, 5.41%) topologies and symmetry-enforced band nodes (846, 7.35%). These materials provide an important platform for further theoretical and experimental exploration of phonon band topology. For instance, AgP_2 is an efficient and stable CO_2 reduction catalyst, while $KBiO_3$, with its topological nodal line of $Z2$-monopole charge, serves as a visible-light-driven photocatalyst capable of degrading various organic pollutants.

This database provides essential theoretical guidance for exploring the effects of TPs and their surface states on phonon catalysis in catalytic reactions. For surface reactions occurring within the topmost layers of a crystal, TPs can directly interact with reactants during adsorption, desorption, and energy transfer, aiding in overcoming activation barriers and facilitating chemical bond formation or dissociation. This vibrational assistance is particularly crucial during rate-limiting steps in catalytic reactions. Furthermore, phonons can alter the surface structure of catalytic materials, leading to surface reconstruction and change in the availability of active sites. These changes optimize the reaction pathway, improving both selectivity and product yield. Importantly, combining quantum chemistry with high-throughput computational methods reduces computation time and minimizes mapping issues, thereby accelerating the discovery of TP materials.

TOWARDS NEW FUNCTIONAL ENERGY MATERIALS

Beyond topological classification, the establishment of a TP database not only facilitates the analysis of phonons' impact on the physical properties but also enables the study of their influence on catalysis from a chemical perspective. The absence of time-reversal symmetry, for instance, results in phonon states with non-zero Chern numbers, giving rise to the phonon Hall effect, which can be harnessed for the development of phonon diodes and acoustic waveguides. Similarly, the absence of spatial inversion symmetry leads to valleys with non-zero Berry phases, resulting in the valley phonon Hall effect, which has potential applications in phonon valley filters, phononic antennas, and more. It is also essential to emphasize that phonons, as quantized energy packets associated with lattice vibrations, carry both heat and sound. This opens up numerous applications in areas such as thermal conduction, heat capacity, and lattice thermal expansion. In thermoelectrics, for example, the unique edge states and nontrivial band structures of TPs can enhance electrical conductivity while reducing phonon scattering, thereby optimizing both thermal and electrical conductivities and improving thermoelectric performance. Additionally, the robust edge states provide precise control over phonon transport, allowing for better heat flow direction and improved thermal management. Compared to traditional thermoelectric materials, the stable phonon modes of TPs can enhance material stability, ensuring consistent thermoelectric performance at high temperatures. This paves the way for the development of new materials with lower thermal conductivity and higher thermoelectric efficiency, expanding the possibilities for more efficient thermoelectric materials.[5] Moreover, topological phononic materials also hold promise for topological superconductivity and the engineering of novel phonon devices exhibiting anomalous heat transport.

The creation of this database also provides a foundation for exploring the interaction between topological electrons and TPs within the same material. TPs can transfer the heat generated by the resonant coupling within the catalyst to adjacent units, minimizing energy loss, accelerating molecular bond breaking, and lowering the Gibbs activation energy. This enhances mass transfer and increases the reaction rates. The TP database will enable researchers to better understand the mechanism behind electron-phonon catalysis, control the reaction processes, and manage intermediate products more effectively.

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DECLARATION OF INTERESTS

The authors declare no competing interests.