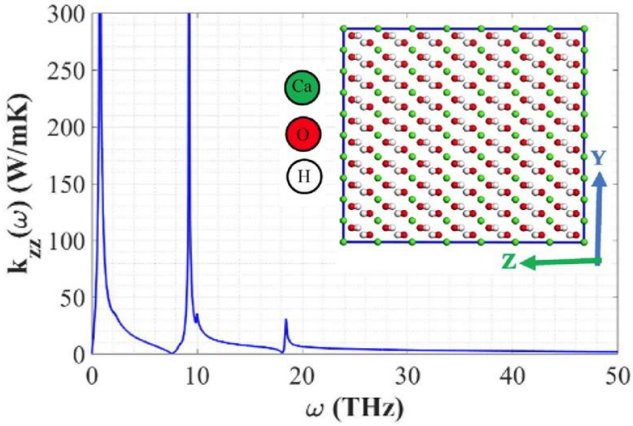
HEAT TRANSPORT THROUGH PORTLANDITE MOLECULE

Live near the sky, a dream made successful by massive concrete infrastructure in cities, also enabling masses to live in a small place. The vibrancy of current lives is now been affected by overheating issues caused by the tall buildings obstructing the free air pass creating an urban heat island. Excessive energy consumption for cooling indoors gives rise to economic challenges.

Several front strategies are needed to mitigate the issue. A re-engineered application of the material, especially cement has become a point of interest in the scientific community. Detailed knowledge about the structure-property relationship of components of cement glue might give the proper key for advancement. Thermal transport mechanism through portlandite at the molecular scale level [Sarkar et al. "Thermal conductivity of Portlandite: Molecular dynamics based approach". Cement and Concrete Res.; https://doi.org/10.1016/j.cemconres.2023.107347] is a notable research in this regard.

A simulation-based study in the framework of molecular dynamics on portlandite reveals the quantitative participation of its different molecular groups in thermal transport. The study has adopted three commonly used force fields (ClayFF, IFF, and ReaxFF) for a thorough investigation of both thermal conductivity value and the transport mechanism alongside experiments based on modulated differential scanning calorimetry (MDSC).



Contribution of different molecular frequencies for transporting thermal flux along the Z direction in portlandite crystal

The study has been summarised with computational outcomes which are observed to be very sensitive to the force field, emphasizing that the validity of the force fields is property-dependent. Besides, thermal properties, mechanical and vibrational properties have also been investigated. Interestingly the thermal conductivity turns to be controlled by boson-peak excitations.

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MIRACLE Photonic Concrete

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