A Survey of Theoretical Methods for Predicting the Thermal Properties of Materials

M. Hussein N. Assadi

[1] *School of Materials Science and Engineering, The University of New South Wales, NSW 2052, Australia.*

The successful utilisation of fusion energy requires multiple breakthroughs in several allied disciplines. One of the most pressing issues is the reliable prediction of the thermal response of the components under extreme conditions. Consequently, having accurate knowledge of materials' anticipated high-temperature thermal behaviour based on condensed matter theories becomes indispensable for successful fusion reactor design. The thermal response of crystalline materials can be understood by the vibration of atoms around their equilibrium positions, referred to as phonons [1]. *Ab initio* knowledge of phonons' behaviour can predict quantities such as thermal expansion coefficients, heat capacity, and thermal conductivity of a given material [2].

This presentation reviews the recent developments in calculating phonon-related solids' properties based on density functional theory and force fields based lattice dynamics calculations. We also discuss each method's strengths and shortcomings, paying particular attention to the computational costs, parallelisation efficiency, and accuracy of the calculated properties. Specifically, modern tools such as the *Alamode* package [3] for harmonic and anharmonic phonon calculations and the *Compressive Sensing Lattice Dynamics* method [4] and package is reviewed. Furthermore, recent advances in developing highly accurate force fields based on density functional calculations and machine learning as implemented in the *PyXtal_FF* code [5] is discussed. Finally, new frontiers in calculating phonon related properties based on highly efficient tight-binding density functional theory are put forward.

References

[1] J.J. Gutiérrez Moreno et al. *Mater. Renew. Sustain. Energy* **9** 16 (2020).

[2] H.A. Eivari et al. *Mater. Today Energy* **21** 100744 (2021).

[3] T. Tadano et al. *J. Phys.: Condens. Matter* **26** 225402 (2014).

[4] F. Zhou et al. *Phys. Rev. B* **100** 184308 (2019).

[5] H. Yanxon et al. *Mach. Learn.: Sci. Technol.* **2** 027001 (2021).