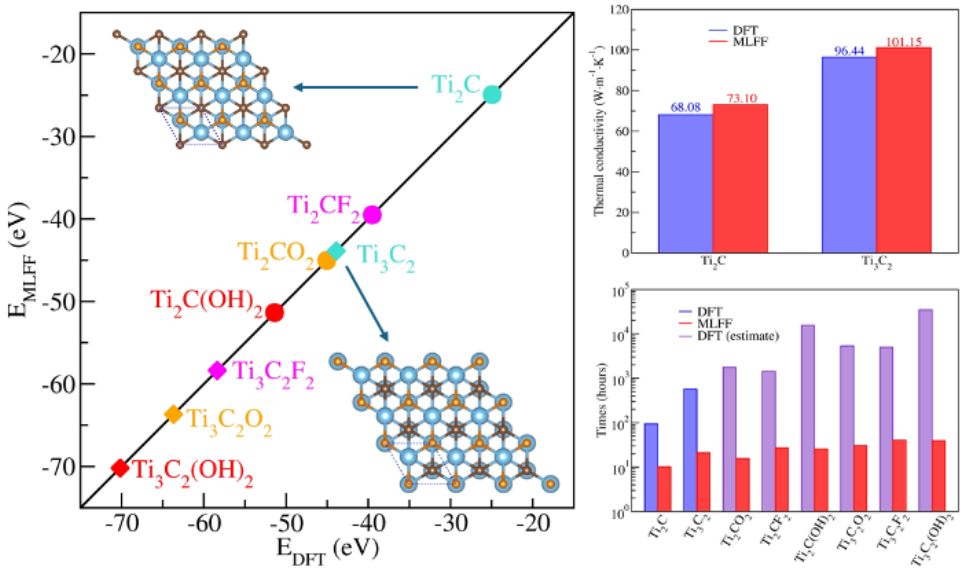
# Smart Simulations: On-the-Fly Machine Learning Force Fields for Lattice Thermal Conductivity in 2D Materials

Thanasee Thanasarnsurapong,[1] Panyalak Detrattanawichai,[2] and Adisak Boonchun*[1]

[1] *Department of Physics, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand; adisak.bo@ku.th*
[2]*Department of Materials, Imperial College London, London SW7 2AZ, United Kingdom*

Traditionally, lattice thermal conductivity is evaluated using the phonon Boltzmann transport equation (PBTE) in combination with Density Functional Theory (DFT) calculations. However, this approach is computationally intensive. In this study, we predicted the lattice thermal conductivity of $Ti_2C$ and $Ti_3C_2$ MXenes, as well as $MoS_2$, using active DFT-based on-the-fly Machine Learning Force Fields (MLFF). Our results reveal that the MLFF-predicted thermal conductivities of MXenes and transition metal dichalcogenides (TMDs) closely match DFT-calculated values. Furthermore, we demonstrate the application of MLFF in studying the impact of surface functional groups (O, H, and OH) on lattice thermal conductivity. A key finding is that MLFF-based predictions are tens to thousands of times faster than conventional DFT calculations, significantly accelerating the study of thermal transport in MXenes. This efficiency highlights the potential of MLFF as a powerful tool for exploring and optimizing the thermal properties of two-dimensional materials..




## References

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2. Jinnouchi, R.; Karsai, F.; Kresse, G. *Physical Review B*, **2019**, 100, 014105.