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# Development and application of ALAMODE software

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{\it Ab initio} phonon calculation plays an essential role in the modern computational materials science study, which aims to predict and elucidate thermodynamic and transport properties of materials at finite temperature. The harmonic approximation in phonon calculation is very useful and has been successful for many materials. However, it naturally fails to describe anharmonic properties and often breaks down in many energy- and light-harvesting materials. Therefore, developing a more accurate and versatile phonon calculation method that can handle strong anharmonicity is vital.

To overcome the limitation of the conventional phonon calculation method, we have been developing the \textsc{alamode} [1], an opensource software for anharmonicity and thermal transport. In this talk, I will present several features of \textsc{alamode}, including the self-consistent phonon calculation [2] and the efficient estimation of force constants [3,4], as well as its applications to thermoelectric materials [5] and ceramics [6].

Refs
[1] https://github.com/ttadano/alamode
[2] T. Tadano and S. Tsuneyuki, Phys. Rev. B {\bf 92}, 054301 (2015); J. Phys. Soc. Jpn. {\bf 87}, 041015 (2018).
[3] F. Zhou, W. Nielson, Y. Xia and V. Ozoliņš, Phys. Rev. Lett. {\bf 113}, 185501 (2014).
[4] https://alm.readthedocs.io/en/develop/
[5] T. Tadano, Y. Gohda and S. Tsuneyuki, Phys. Rev. Lett. {\bf 114}, 095501 (2015); T. Tadano and S. Tsuneyuki, Phys. Rev. Lett. {\bf 120}, 105901 (2018).
[6] Y. Oba, T. Tadano, R. Akashi and S. Tsuneyuki, Phys. Rev. Materials {\bf 3}, 033601 (2019).

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