Contribution ID : 111 Type : Oral

Ab initio structural optimization at finite temperatures based on anharmonic phonon theory

Tuesday, 24 September 2024 11:25 (30)

In this presentation, I will report on the development of first-principles structural optimization at finite temperatures and their applications. At zero temperature, structural optimization commonly involves minimizing the energy of the system based on density functional theory. However, it is necessary to consider minimizing the free energy at finite temperatures. In doing so, it is essential to consider the contributions of phonons, including anharmonic terms. We have formulated a method based on anharmonic phonon theory. In particular, we developed a technique for efficiently evaluating the interatomic force constant, which we applied to BaTiO3 and LiBO3 (B=Ta, W, Re, Os). Our method has been found to accurately evaluate the experimental transition temperatures of structural phase transitions in both insulators and metals.

[1]R. Masuki, T. Nomoto, R, Arita, and T. Tadano, Phys. Rev. B 106. 224104 (2022)
[2]R. Masuki, T. Nomoto, R, Arita, and T. Tadano, Phys. Rev. B 110, 094102 (2024)

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Session Classification : Session