Contribution ID: **157** Contribution code: **S2 Condensed Matter Physics** Type: **Oral Presentation**

First principles study on thermal conductivity of nitrogen substituted diamane

Friday 24 June 2022 15:00 (15 minutes)

Over the last decade since the discovery of graphene, two-dimensional materials have gained a great attention due to their outstanding properties suitable for fabrication of next generation nanodevices. A single-layered diamond or diamane, whose high stiffness and high thermal conductivity are inherited from its bulk counterpart, is a candidate for heat dissipating device applications. Unfortunately, pristine diamane is structurally unstable without passivation of dangling bonds on it surfaces by H, F, and OH. Recent theoretical studies have suggested that site-specific substitution of N for C can stabilize the diamane's structure without surface termination. Despite its superhard properties inherited from bulk carbon nitrides, thermal properties of N-substituted diamane have not been explored. In this work, we investigate thermal properties of N-substituted diamane using density functional theory and Boltzmann transport equation in the relaxation time approximation. Our results show that the flexural phonon branch, which is typically observed in two-dimensional materials, appears in the phonon dispersion relation of N-substituted diamane and it contributes large thermal conductivity to the material. Also, we estimate the thermal conductivity of N-substituted diamane as a function of temperature, and the results are discussed in comparison with that diamond.

Author: Mr KHAMKAEO, Sakarn (Chulalonkorn University)

Co-authors: Dr PAKORNCHOTE, Teerachote (Chulalonkorn University); Dr EKTARAWONG, Annop (Chulalongkorn University); Dr BOVORNRATANARAKS, Thiti (Chulalonkorn University)

Presenter: Mr KHAMKAEO, Sakarn (Chulalonkorn University)

Session Classification: S2 Condensed Matter Physics

Track Classification: Condensed Matter Physics