

理論セミナー / Theory Seminar

Date: Feb. 18 (Fri.), 2022 16:00-

Place: On Zoom

Speaker: **Prof. Hisazumi Akai**

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Title: **Effects of electron-phonon and -magnon scattering on the finite temperature magnetization of permanent magnet materials**

Abstract:

For the development of permanent magnet materials, it is crucial to improve their magnetic properties at finite temperature including the Curie temperature. In terms of first-principles electronic structure calculations, these properties are rarely addressed because of the difficulties arising from the itinerant nature of the magnetism of these materials. So far, most attempts have been made to use the nonlocal static susceptibility, calculated by, e.g., according to Liechtenstein's prescription, which is mapped to exchange couplings J 's of the classical Heisenberg model, and to apply statistical methods to it. One of the problems of such approaches is that J 's are actually strongly temperature dependent in the itinerant electron systems is neglected. The effects of electron scattering due to phonons and magnons on J 's are particularly important. In the present study, we include both the effects on electronic structure and hence J 's at moderately high temperatures and discuss finite temperature magnetization and the Curie temperature from first-principles.



<https://forms.gle/itAy8SiBJQPEcWxA7>

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