
7th International Workshop on 2D Materials

Title of the Presentation: Theory of ground and excited states in layered magnetic materials

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Short Biography:

Y.-W. Son received his Ph. D. from Department of Physics, Seoul National University in 2004. After then, he visited UC Berkeley as a post-doctor and was an assistant professor at Physics Department, Konkuk University Seoul Campus. Since 2008, he has been a professor of computational sciences in Korea institute for advanced study, Seoul, Korea. He has interested in theoretical and computational understanding of solids and nanostructures in general.

Abstract:

In this talk, I will present my recent two works related with layered magnetic materials. First, to compute accurate electronic structures of large scale low dimensional systems having both p and d orbitals and to compare their total energies appropriately, we have developed a new first- principles method exploiting self-consistent evaluations of on-site and inter-site Hubbard interactions simultaneously [1]. It turns out that the new method captures a local Coulomb repulsion, covalent hybridization and their coexistence very well. With this, we investigate the ground states of various chromium trihalides compounds [2]. Second, within the configuration interaction theory, we compute resonant inelastic scattering spectroscopic signals for a layered antiferromagnetic NiPS₃ and obtain excellent agreement with an experiment [3]. Based on this, we explore a possible ordering of excitons with a background magnetism that may explain the observed anomalous optical absorptions and photoluminescence [3].

[1] S.-H. Lee and Y.-W. Son, *Phys. Rev. Research* **2**, 043410 (2020)

[2] S.-H. Lee and Y.-W. Son, *in preparation*.

[3] S. Kang, K. Kim, B. H. Kim *et al.*, *Nature* **583**, 785 (2020)