APCTP SEMINAR

Calculation of electronic structure and X-ray spectra for correlated materials

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November 3rd (Wed.) 16:00 (KST)

#512, APCTP HQ

Correlated electrons pose a difficult problem for the standard method used for electronic structure calculations, Kohn-Sham density functional theory (KS-DFT). In order to better deal with this group of materials the DFT+U and DFT + DMFT methods have been developed to include electron-electron correlations in calculating the electronic structure. For calculating the X-ray spectra of correlated materials, a method that combines multiplet ligand field theory with DFT calculations (DFT + MLFT) has been developed, greatly reducing the number of parameters required to calculate the X-ray spectra of correlated materials. In this talk I will present some of my work on the recently discovered high pressure phases of TiPO4,, using DFT + U; the magnetic properties of the MAX phase Mn2GaC, using DFT+DMFT; and the X-ray absorption spectra of CrI3 using DFT + MLFT.

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The APCTP is supported by the Korean Government through the Science and Technology Promotion Fund and Lottery Fund and strives to maximize social value through its various activities.

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