**Toward the Better First-principles Description of Correlated Materials: Old Functionals and New Concepts**

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In this talk, I will try to give a brief overview of recent progress in my research group for developing first-principle-based computation methods. In the first part, I will discuss LDA/GGA+U functionals. Although this method has become a standard tool ever since its first suggestion in 1991, the detailed understanding of the differences in between various functional recipes has not been reached yet which severely hampers the application to real material research. With this motivation, we recently performed the systematic and comparative analysis on this issue [1,2]. In the second part, I will discuss a new physical quantity temporally named as ‘effective degeneracy’ or ‘effective entropy’. In understanding condensed matter systems, it is sometimes crucially important to develop or define a new physical concept which carries the key physical intuition. In order to understand multi-band Mott transitions, we suggest this quantity based on entropy-like term [3]. Its usefulness will be demonstrated with some materials examples. Finally (if time allows), I will also introduce our recent developments for the magnetic force linear response calculation techniques [4] as well as the new analytic continuation methods [5, 6].

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6. H. Yoon et al., arXiv:1806.03841 (submitted).