量子物理学・ナノサイエンス第 454 回セミナー

Pushing the limits of density-functional theory for accurate and predictive simulations of complex materials

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場所　：　本館 2 階 227B 物理学系輪講室

概　要

Density-functional theory (DFT) is one of the most widely used first-principles theoretical frameworks for understanding and predicting the properties of materials. For systems containing localized electronic states, Hubbard-corrected functionals provide an efficient extension of DFT that can substantially improve the description of electronic structure, energetics, and magnetic properties. In this seminar, I will present a decade of theoretical developments aimed at making Hubbard-corrected DFT more predictive, systematic, and broadly applicable. I will introduce our approach for calculating on-site U and inter-site V Hubbard parameters self-consistently and from first principles using density-functional perturbation theory [1,2,3]. I will discuss how these developments have been incorporated into DFT+U and DFT+U+V and implemented in the open-source Quantum ESPRESSO suite [4]. I will then illustrate applications to a range of problems in condensed matter and materials physics, including transition-metal oxides, battery materials, defects in perovskites, and photocatalysts. Examples will cover structural and electronic properties, voltages, formation energies, band gaps, and magnetic properties, with comparisons between theoretical predictions and available experimental results. Finally, I will discuss recent extensions of these approaches beyond static ground-state calculations, including lattice dynamics, electron-phonon coupling, and magnetic excitations. Throughout the talk, I will emphasize the theoretical foundations of the methods, their practical implementation, and the connection between computational predictions and experimentally measurable properties. The goal is to provide a perspective on how systematic developments of Hubbard functionals can turn DFT-based calculations into more reliable quantitative tools for studying complex materials.

[1] I. Timrov, N. Marzari, M. Cococcioni, Phys. Rev. B **98**, 085127 (2018).
[2] I. Timrov, N. Marzari, M. Cococcioni, Phys. Rev. B **103**, 045141 (2021).
[3] I. Timrov, N. Marzari, M. Cococcioni, Comput. Phys. Commun. **279**, 108455 (2022).
[4] P. Giannozzi *et al.*, J. Phys.: Condens. Matter **29**, 465901 (2017).

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