



復旦大學
FUDAN UNIVERSITY

Applied Math Ph.D. Seminar

Fast Generation of Pipek-Mezey Wannier Functions via the Co-Iterative Augmented Hessian Method

Speaker: Gengzhi Yang (University of Maryland)

Time: 2026-05-28, 15:10 to 16:00

Location: Rm 1801, Guanghai East Tower

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Abstract: We report a k -point extension of the second-order co-iterative augmented Hessian (CIAH) algorithm, termed k -CIAH, for Pipek–Mezey (PM) localization of Wannier functions (WFs). By exploiting an efficient evaluation of the Hessian–vector product, k -CIAH achieves $O(N_k^2 n^3)$ scaling in both CPU time and memory, matching that of previously reported first-order k -space approaches while improving upon the $O(N_k^3 n^3)$ scaling of Γ -point CIAH, where N_k denotes the number of k -points sampling the first Brillouin zone and n characterizes the unit-cell size. Benchmark calculations on a diverse set of solids—including insulators, semiconductors, metals, and surfaces—demonstrate the fast and robust convergence of k -CIAH-based PMWF optimization, which yields an overall computational efficiency approximately 2–3-fold higher than first-order k -space methods and orders of magnitude higher than Γ -point CIAH for localizing 1000–5000 orbitals. The quality of the resulting PMWFs is further validated by accurate electronic band structures obtained via PMWF-based Wannier interpolation.