Gaussian-based Quantum Chemistry for Materials Science

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I will present our recent work on a series of methodological and algorithmic developments in the PySCF code for simulating condensed-phase materials using periodic quantum chemistry with Gaussian basis functions. Our developments address two key challenges in such simulations: the evaluation and storage of the electron-repulsion integrals [1,2,3] and the generation of high-quality Gaussian basis sets [4]. As a demonstrative application, I will show the calculation of the cohesive energy of the benzene crystal in both the thermodynamic limit and the complete basis set limit using fully periodic second-order Møller-Plesset perturbation theory, where the largest calculation correlates about 500 electrons in more than 16,000 basis functions. These advances will facilitate the routine application of quantum chemistry methods, which have been widely used in computational molecular science research, to practical computational materials science research.

[1] Ye and Berkelbach, JCP, 154, 131104 (2021).
[2] Ye and Berkelbach, JCP, 155, 124106 (2021).
[3] Ye and Berkelbach, submitted (arXiv:2206.01801).
[4] Ye and Berkelbach, JCTC 18, 1595 (2022).