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Speeding up GW Calculations for Large Scale Quasiparticle Predictions[1] WEIWEI GAO, WEIYI XIA, State Univ of NY - Buffalo, XIANG GAO, Beijing Computational Science Research Center, PEIHONG ZHANG, State Univ of NY - Buffalo — Although the GW approximation is recognized as one of the most accurate theories for predicting materials excited states properties, scaling up conventional GW calculations for large systems remains a major challenge. We present a powerful and simple-to-implement method that can drastically accelerate fully converged GW calculations for large systems, enabling fast and accurate quasiparticle calculations for complex materials systems. We demonstrate the performance of this new method by presenting the results for bulk and 2-dimensional systems. A speed-up factor of nearly two orders of magnitude is achieved for large systems.

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