Efficient large-scale GW calculations for 2D materials[1] WEIYI XIA, WEIWEI GAO, YABEI WU, PEIHONG ZHANG, State Univ of NY - Buffalo — Accurate and efficient predictions of excited-states properties of complex materials remain a major challenge due to complication of the convergence issue and the unfavorable scaling of the computational cost with respect to the system sizes. GW calculations for 2D materials pose additional challenges due to the analytical behavior of the 2D dielectric function. Recently we have developed a powerful method [1] that can drastically improve the speed of GW calculations for large systems. In this work, we apply this newly developed method to study the quasiparticle band structure of recently synthesized layered material C2N [2] which contains 18 atoms for the single layer system. We will discuss the convergency behavior of the calculated quasiparticle band structure with respect to the k-point sampling density and the number of bands included in the calculations of the dielectric function and the Coulomb-hole self-energy, aiming at shedding some light on accurate and efficient GW calculations for two-dimensional materials. [1] W. Gao, W. Xia, X. Gao, and P. Zhang, in press, Scientific Reports (2016). [2] J. Mahmood et al, Nat Commun. 6, 6486 (2015).

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