

Supplementary information

Vertical Dielectric Screening of Few-Layer van der Waals Semiconductors

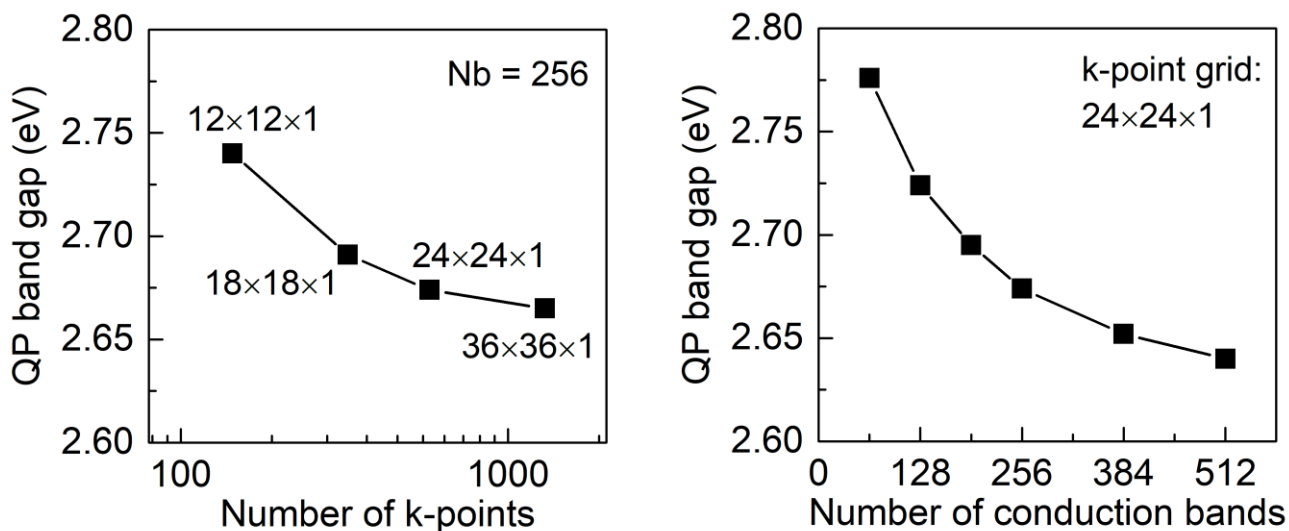
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The convergence of the GW calculation:



We use the single-shot GW calculation implemented in the BerkeleyGW package. The dynamic screening is based on the Plasmon-pole model, which has been shown to be reliable to obtain quasiparticle bandgap of two-dimensional semiconductors [1, 2]. The convergence test of monolayer MoS₂ is presented in the above figures. For the left panel, we fix the number of conduction bands and increase the k-point sample density. For the right panel, we fix the k-point sampling grid to be 24×24×1 and increase the number of conduction bands. Both tests show that our setting parameters (24×24×1 k-point sample and 256

conduction bands) can give an error bar of the quasiparticle band gap within 0.1 eV. Finally, we find that the quasiparticle band gap is not very sensitive to the energy cutoff of the dielectric function, and we set it to be 15 Ry.

References:

[1] Ashwin Ramasubramaniam, Phys. Rev. B 86, 115409 (2012)

[2] Diana Y. Qiu, Felipe H. da Jornada, and Steven G. Louie, Phys. Rev. Lett. 111, 216805 (2013).