

---

# Accurate band gaps of extended systems via efficient vertex corrections in GW

Wei Chen<sup>1</sup>, Alfredo Pasquarello<sup>1</sup>

1) *Ecole Polytechnique Federale de Lausanne (EPFL)*

Corresponding author: Wei Chen (wei.chen@epfl.ch)

---

Accurate determination of band gaps of extended systems remains challenging within the framework of GW. Notably, the quasiparticle self-consistent GW systematically overestimates the band gaps as a result of the neglect of vertex corrections in the screening. Here we propose the use of an efficient bootstrap exchange-correlation kernel to account for the vertex corrections in self-consistent GW calculations. The approximate kernel leads to accurate band gaps for various extended systems, including simple sp semiconductors, wide band-gap insulators, and 3d transition-metal compounds. The accuracy is compatible with that obtained via the solution of the Bethe-Salpeter equation, making the method particularly useful for band-gap predictions of large-scale systems.