# A computational method for ARPES based on

# repeated slab DFT calculations

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In this work, we developed a computational method for constructing photoelectron wave functions from Kohn-Sham orbitals obtained by DFT calculations.

Also, we calculated photon energy dependence of photoemission intensity from graphene monolayer with the matching method and confirmed that the results agreed well with the results of multiple scattering calculations. We expect that this method enable quantitative and efficient prediction of photoelectron spectra in various thin film systems.
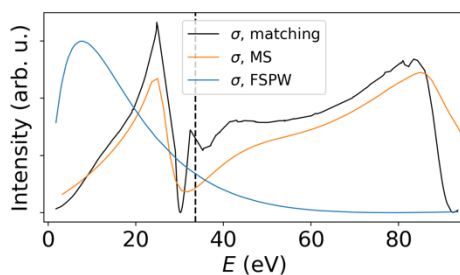
**Figure 1** Normal photoemission intensity emitted from $\sigma$ state of graphene（black: matching method, orange: multiple scattering method, blue: final state plane wave approximation）.