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Exchange self-energy and compressibility of multilayer graphene by wavefunction rotation method[1] HONGKI MIN, Seoul Natl Univ — Multilayer graphene has chiral electronic structure which strongly depends on the stacking sequence. A fundamental issue is to understand the interplay between the chiral electronic structure and electron-electron interaction, and the exchange interaction is the leading-order correction to the electron-electron interaction. The exchange energy calculation of multilayer graphene, however, requires a large amount of computational cost, because of non-local nature of the exchange interaction and because of the absence of the analytic form of the wavefunction, which should be obtained self-consistently. We overcome this problem using the wavefunction rotation method, in which the angular part of the wavefunction is obtained analytically by attaching a phase factor that is determined by the stacking sequence, thus reducing the computational cost significantly. Using this method, we calculate the exchange self-energy and compressibility of multilayer graphene, and discuss the role of intralayer and interlayer exchanges.

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Hongki Min
Seoul Natl Univ

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