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Interlayer Binding of Bilayer α-graphyne : Quantum Monte Carlo Study YONGKYUNG KWON, HYEONDEOK SHIN, HOONKYUNG LEE, Konkuk University, JEONGNIM KIM, Oak Ridge National Laboratory — Graphynes have recently received considerable attention because of their intriguing potential as new Dirac materials. Recent DFT calculations of Leenaerts *et al.* [1] predicted two stable stacking modes of bilayer α-graphyne; while a AB-stacked configuration was found to possess a gapless parabolic band structure, the other stable mode of Ab-stacked graphyne exhibits a double Dirac cone spectrum. On the other hand, more accurate DFT calculations predicted different ground-state configurations for bilayer α-graphyne, depending on the van der Waals (vdW)-corrected exchange-correlation functional used. In order to determine the most stable configuration of bilayer α-graphyne along with accurate computation of its interlayer binding energy, we here employ quantum Monte Carlo method which allows accurate description of the vdW interaction between two graphyne layers. The QMC results for the interlayer binding energies have revealed that the Ab-stacking mode is slightly favored than the AB mode but the binding energy difference is very small, only about 0.3 meV/atom. It is also found that the DFT results with vdW-DF2, based on the non-local vdW functional proposed by Lee *et al.* [2], are in good agreement with the QMC results. This leads us to conclude that within the DFT formalism the interlayer binding of the graphyne structures is best described by the vdW-DF2 functional. [1] O. Leenaerts *et al.*, Appl. Phys. Lett. **103**, 013105 (2013). [2] K. Lee *et al.*, Phys. Rev. B **82**, 081101R (2010).

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