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Interlayer Binding of Bilayer Low-dimensional sp,sp^2- Hybridized Carbon Networks : Quantum Monte Carlo Study[1] HYEONDEOK SHIN, Argonne Natl Lab, JEONGNIM KIM, Intel Corporation, ANOUAR BENALI, Argonne Natl Lab, YONGKYUNG KWON, Konkuk University — We have performed the quantum Monte Carlo(QMC) method to study interlayer binding of a bilayer α-graphyne. A sp,sp^2-hybridized α-graphyne have been received a great deal of attention due to its unique electronic properties compared with that of graphene. However, since the most stable mode in the DFT framework was varied along applied vdW-corrected correlation functionals, the most favored mode for a bilayer α-graphyne was not confirmed.[1] Our QMC calculations confirmed the most favored mode for a bilayer α-graphyne and revealed that vdW-corrected DFT binding energies significantly underestimate interlayer bindings of sp,sp^2-hybridized carbon network systems while overestimations within corresponding DFT functionals were observed in a graphene in recent QMC studies.[2] Among vdW-corrected DFT functionals, the rVV10 functional described the most consistent interlayer geometries with QMC ones for low-dimensional carbon allotropes, however, completely misestimated charge density distribution within the rVV10 yields significant quantitative discrepancy of interlayer binding energies between QMC ones. [1] O. Leenaerts *et al.*, Appl. Phys. Lett. **103**, 013105 (2013). [2] E. Mostaani *et al.*, Phys. Rev. Lett. **115**, 115501 (2015).

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