Quantum Monte Carlo calculation of sp-bonded carbon chains: carbynes and carbon rings IUE GYUN HONG, JEONGHWAN AHN, HYEONHU BAE, KonKuk Univ, HYEONDEOK SHIN, Argonne National Laboratory, SUNGJIN PARK, HOONKYUNG LEE, KonKuk Univ, ANOUAR BENALI, Argonne National Laboratory, YONGKYUNG KWON, KonKuk Univ, DEPT. OF PHYSICS, KONKUK UNIVERSITY, SEOUL 05029, KOREA TEAM, LEADERSHIP COMPUTING FACILITY, ARGONNE NATIONAL LABORATORY, ARGONNE, IL 60439, U.S.A COLLABORATION — Both density functional theory (DFT) and quantum Monte Carlo (QMC) methods have been employed to study ground state properties of two forms of sp-bonded carbon chains: carbynes and carbon rings. According to the DFT-PBE calculations, polyyne, a carbyne structure with alternating single and triple C-C bonds, is energetically favored by 14 meV/atom over cumulene only with double bonds. However, our QMC calculations predict an energy difference of 88(4) meV/atom between them, clearly demonstrating that polyyne is the ground-state structure of carbyne. In the study of carbon rings consisting of 4n and (4n+2) C atoms, DFT calculations show electrons to be delocalized even in the regime where dimerization effects should be large. In contrast, for n¿4, QMC calculations indicate the greater stability of a Peierls insulator configuration over a ground state predicted by Huckels rule. This qualitative difference between QMC and DFT results shows that many-body correlation effects taken into account by the QMC method are necessary to accurately describe even simple carbon systems such as sp-bonded carbon chains.

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