Prediction of carbon clusters using machine-learning potential

Huy Duy Nguyen
University of Science, Vietnam National University, Hanoi, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam
Email: huydn@hus.edu.vn

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In our investigation of twelve-atom carbon clusters, we employ the recently developed machine-learning potential GAP-20 to predict the low-energy isomers. The GAP-20 model exhibits good agreement with density-functional theory calculations for most isomers, accurately capturing geometric structures and average C-C bond lengths. However, the GAP-20 significantly underestimates the energies associated with cage-like structures, leading to an incorrect ground state prediction. The Jahn-Teller distortion associated with the monocyclic ring is also absent. This intriguing behavior prompts further exploration. Comparing cohesive energies, the GAP-20 performs well for monocyclic rings. In addition, it also reveals two novel low-energy isomers composed of multicyclic rings. These previously undiscovered structures challenge our existing understanding and open up exciting avenues for future research. The GAP-20 provides valuable insights into the intricate landscape of carbon clusters by shedding light on these multicyclic configurations.

Keywords: Carbon clusters, Low-energy isomers, Machine-learning potential