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Pseudopotential Density-Functional Calculations for Structures of Small Carbon Clusters C_N (N=2～8)

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Abstract: We introduce a first-principles density-functional theory, i.e. the finite-difference pseudopotential density-functional theory in real space and the Langevin molecular dynamics annealing technique, to the descriptions of structures and some properties of small carbon clusters (C_N, N=2～8). It is shown that the odd-numbered clusters have linear structures and most of the even-numbered clusters prefer cyclic structures.

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