

Length- and parity-dependent electronic states in one-dimensional carbon atomic chains on C(111)

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Using first-principles density-functional theory calculations, we find dramatically different electronic states in the C chains generated on the H-terminated C(111) surface, depending on their length and parity. The infinitely long chain has π electrons completely delocalized over the chain, yielding an equal C-C bond length. As the chain length becomes finite, such delocalized π electrons are transformed into localized ones. As a result, even-numbered chains exhibit a strong charge-lattice coupling, leading to a bond-alternated structure, while odd-numbered chains show a ferrimagnetic spin ordering with a solitonlike structure. These geometric and electronic features of infinitely and finitely long chains are analogous to those of the closed (benzene) and open (polyacetylene) chains of hydrocarbons, respectively.