

Public Abstract

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Title:The Use of Polyhedral Derivatives as Molecular Electronic Scaffolds

Electronic devices, such as cell phones and computer chips, are becoming smaller in size and more complex in their abilities. Currently, engineering the construction of smaller electronic components that have sufficient ability is quite challenging. This work suggests the use of a single molecule for electronic components, rather than using the current method of a large array of molecules. This significantly reduces the size without sacrificing ability. To this end a single scaffold, dodecaborate, was computationally modeled to examine its ability to function in an electrical circuit. Additionally the question of fundamentally where the electrons, or electric current, would be contained was addressed. Dodecaborate is a three – dimensional polyhedral borane that contains 26 "free" electrons, which were found to be able to become coupled to other electrical components. Several derivatives were systematically tested to highlight the versatility of dodecaborate as a scaffold for a variety of electronic devices, specifically transistors and rotors. Furthermore, this work puts an impetus on molecular electronics as next - generation technology.