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Theoretical studies of energetic stability and electronic properties of fullerene derivatives and their solid forms

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Abstract (Summary)

Two types of new forms of carbon that are based on fullerene units and exhibit properties similar to those of diamond are investigated. The first are solids formed from $\rm C\sb{28}$ clusters arranged in three variants of the diamond lattice. The energetics and electronic properties of these three lattices are compared and analyzed in detail. Secondly, we discuss a new class of carbon clusters which exhibit tetrahedral bonding that we have proposed recently. The structural and electronic properties of these clusters, as well as those of their hydrogenated and solid forms, are described.

Using ab initio electronic structure calculations, we study several cluster assembled forms of carbon which are based on $\rm C\sb{28}$ units. First, we investigate how the charge density and electronic spectrum of an isolated $\rm C\sb{28}$ unit is altered when these units are arranged in a diamond crystal, called hyperdiamond. We analyze the nature of electronic states near the Fermi level of both an isolated $\rm C\sb{28}$ cluster and of hyperdiamond. We next focus on two new solids, called $\rm C\sb{28}C$ and $\rm C\sb{28}Si,$ based on the $\rm C\sb{28}$ unit plus an additional single carbon or silicon atom arranged in a zincblende lattice. We show that these two new solids are energetically preferred to hyperdiamond. We analyze the electronic states of $\rm C\sb{28}C$ and $\rm C\sb{28}Si$ in detail, and make comparisons to those of hyperdiamond and diamond. The role of additional intercluster interactions found in $\rm C\sb{28}C$ and $\rm C\sb{28}Si$ that are not found in $(\rm C\sb{28})\sb2$ is discussed.

In addition to studying diamond-like lattices built from $\rm C\sb{28}$ units, we also examine new forms of carbon based on individual fullerene units that have diamond-like structure. We investigate the properties of a new class of structures consisting of compact carbon clusters with surface threefold coordination and bulk fourfold coordination. These clusters are the diamond analogues of fullerenes, maintaining almost perfectly tetrahedral bonding and icosahedral symmetry. Two potentially stable forms are investigated: molecules with hydrogenated surfaces and solid close-packed arrangements. We use bond energies and electronic structure calculations to examine the relative stability of various sized clusters in both hydrogenated and pure form.

Indexing (document details)

Advisor:	Kaxiras, Efthimios
School:	Harvard University
School Location:	United States -- Massachusetts
Keyword(s):	diamond lattice, carbon clusters
Source:	DAI-B 55/08, p. 3393, Feb 1995
Source type:	Dissertation
Subjects:	Condensation
Publication Number:	AAT 9500169
Document URL:	http://ezp1.harvard.edu/login?url=http://proquest.umi.com.ezp-prod1.hul.harvard.edu/pqdweb?did=741082881&sid=17&Fmt=2&clientId=11201&RQT=309&VName=PQD
ProQuest document ID:	741082881

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