Structural Models of Alkali Metal Atom

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Introduction

Alkali metals belong to the s-block elements on the leftmost side of the periodic table. Alkali metals lose electronsmaking them the most reactive elements on earth. Electronic configurations, ionizatifon enthalpy, hydration enthalpy and atomic, ionic radii, and other physical and chemical properties of the group one alkali metals are discussed below.Structural models of alkali metal atoms are proposed to be doped with less than about 0.1 potassium or rubidiumatoms per carbon.These alkali metals are used to be expanded through a supersonic nozzle.These models utilize a basic motif of an alkali metal column surrounded by four zig zag polyacetylene chains.In these stage 2 models each chain of polyacetylene chain,they have only one alkali metal column neighboring them.

Literature

Alkali metals occupy the first column of the periodic table. They are very reactive and are present in form of compounds containing one electron in their valence shell. The nuclear charge increases and a new orbital gets added to each alkali atom. Every alkali metal has the largest radii of any other element in the corresponding period.These have the lowest density having the largest radius and volume.Compounds of carbon are present in every object used in daily life.C60 sphere, fullerenes are highly symmetrical and have a similar structure to graphite.Cylindrical fullerenes are also known as nanotubes. C_{60} is the most common fullerene having no two pentagons sharing the same edge. A C_{60} molecule's average carbon-carbon bond length is 1.44 angstrom. The fullerenes, especially the C_{60} sphere, excite the imagination of scientists as they bridge gaps between the sciences, architecture, mathematics, engineering, and the visual arts.Earlier only two well-defined allotropes of carbon were known—diamondand graphite. The fullerenes are the third form,

and it is noticeable that their existence conquered discovery until almost the end of the 20th century. Their discovery gave birth to a new meaning of sheet materials, and it has opened a new chapter of nanoscience and nanotechnology at the atomic scale that exhibits advanced materials behavior. Nanotubes, particularly exhibit a wide range of novel mechanical and electronic properties. They are very good conductors of heat and electricity.

Scope

Presentlystudies are available tonic state, lattice constant, bulk modulus, and phonon dynamics of alkali doped C_{60} solid compound carbons. The diameter of the C_{60} molecule is 7.10 in the mean. At room temperature, the C_{60} molecules crystallize into a van der Waals FCC solid having value of 14.17 Å. The C_{60} molecule is almost incompressible whereasthe molecular solid is quite compressible. Since the C_{60} molecule is large, they have large enough cavities at tetrahedral and octahedral sites, which can collect dopants. Alkali metals and alkaline earth metals are the most studied dopants as these solids are superconductors. Alkali metal gets ionized as it is doped in C_{60} solid. The electrons released from alkali metal can either form an electron gas or get transferred to C_{60} forming an ionic solid. There is another possibility that some of the electrons may form electron gas and the rest may get transferred to C_{60}. There is a wide disparity in cohesive/Madelung energy calculations also. Schulte and Bohm have objected to the possibility of complete transfer of charge and thus to the formation of K_3C_{60} as an ionic solid. But various experiments have verified K_3C_{60} as a stable ionic system. Not only K_3C_{60} but total charge transfer takes place in K_6C_{60} also. However, givenon-shell Coulomb repulsion, this is even less likely. Therefore it becomes pertinent to inquire about the ionic state of the C_{60} molecule in alkali-doped solids. In doped C_{60} solids, there is little overlap between molecular wave functions on neighboring C_{60}, so the electrons are practically localized on the C_{60} shell. The alkali metal atoms are completely ionized. This leads one to believe that in alkali doped C_{60} solids interactions should be van der Waals and screened Coulomb type. A model has been proposed which takes into account these interactions and thus establishes the ionicity of these solids. Theissue of charge transfer is more interesting in Na doped solids, where Na

forms clusters on octahedral sites with high concentrations of Na. The importance of orientation has also been investigated. The calculations have been done foralmost all alkali metals doped in different stoichiometries.Phonon dynamics and thus thermodynamics of the compounds in MC_{60} Stoichiometry have been done as it is in the simplest structure. We have calculated various thermodynamic quantities such as specific heat, Debye temperature, Gruneisen parameter, thermal expansion, and thermal expansion coefficient.

Conclusion

We conclude that the form of potential and model for ionic solids suggested, gives a fairly qualitative account of lattice dynamical and thermodynamic properties of FCC MC_{60} solid also. The phonon DOS in RbC_{60} (Set-I) presented here resemble qualitatively with neutron scattering results. Thermodynamic quantities obtained here using this model are also expected to be fairly good as there follow from Dos. However, we could not compare the calculations of thermodynamics quantities with experimental values due to the lack of experimental work reported in the literature. In a way, we have reported extensive lattice dynamic and thermodynamic calculation first time for these systems and provideda guideline for future work. We do not expect quantitative agreement of calculated quantities with experimental values as a model of interaction is quite simple. Various interactions between C_{60} and alkali metal are properly incorporated within the framework of RIM. We have found that RIM is fairly good enough compared with RSM. The Debye temperature has also been calculated using specific heat data and found to be close to 60k for all MC_{60} compounds. Except for CsC_{60} Dedye temperature decrease with an increase in the size of alkali metal. Comparing the DOS curve of Set-1 with Set-2 it is clear that alkali metal-carbon interaction playsa significant role in deciding the form of these curves and hence the thermodynamic quantities. Set-2 gives a very good approximation of static properties. It is important to note that, generally alkali metal-doped at the octahedral site does not decide the lattice constant of MnC_{60} solids as earlier explained. Set-2 parameters were obtained by increasing repulsion of octahedral alkali atom-C_{60} and used for MC_{60} stoichiometry compounds only. Since these parameters increase the lattice constant of a compound which is not expected to expand much from the lattice constant of pure C_{60}.

Therefore, it is expected that Set-2 will overestimate the lattice constant of other stoichiometry (MnC_{60}) solids as repulsion has been greatly increased.

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