DYNAMICAL IDENTIFICATION OF A THRESHOLD INSTABILITY IN SI-DOPED HETEROFULLERENES

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Modifying the behavior of fullerenes via the introduction of dopant atoms allows to tailor structural and bonding properties as a function of the impurity identity and content.

In order to achieve this goal we select silicon as dopant atoms, because more than one Si atoms can be contained in the carbon cage. Mass spectroscopy experiments gave clear evidence on the existence of stable Si-doped fullerenes with at least three Si atoms [1] and a value lying in between \( m = 7 \) and \( m = 12 \) (\( m \): the number of Si atoms in the cage) was extracted on the basis of combined mass spectroscopy and photofragmentation data, with \( m = 12 \) taken as the upper limit [2].

Still less conclusive is the estimate of the largest number \( m \) of Si atoms which can replace C atoms in the network without causing its breakdown.

We rationalize the origins of a threshold instability and the mechanism of finite temperature fragmentation in highly Si-doped \( \text{C}_{60}-m\text{Si}_m \) heterofullerenes via a first-principles molecular dynamics approach within density functional theory. We discuss the mechanism by which the Si-doped cage becomes unstable and give the threshold value \( m \) for the number of Si–C replacements.