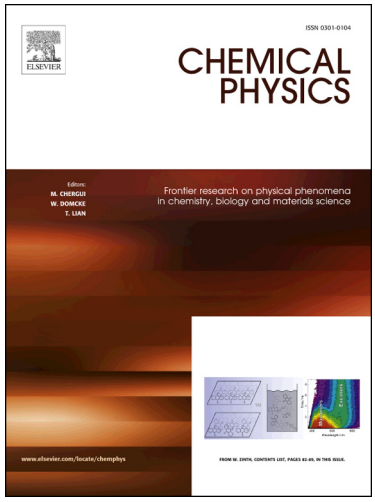

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Jahn-Teller effects and surface interactions in multiply-charged fullerene anions and the effect on scanning tunneling microscopy images

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Abstract

We investigate the combined effects of Jahn-Teller (JT) coupling and interactions with a surface substrate on fullerene anions C_{60}^{2-} to C_{60}^{4-}. JT coupling alone causes the C_{60} ions to instantaneously distort from the icosahedral symmetry of the neutral molecule to a lower symmetry, with the molecule moving dynamically between a set of equivalent distortions. When adsorbed on a surface, the number of equivalent minimum-energy distortions is reduced. The implications of this on observed scanning tunneling microscopy (STM) images will be discussed, and comparisons made with existing experimental data. We show that a consistent interpretation of the images from all of the charge states of C_{60} can only be obtained using a JT model in which the symmetry is further reduced by surface interactions. The comparison with experimental data also allows us to determine relationships between the quadratic Jahn-Teller coupling and surface interaction parameters.

Keywords: Jahn-Teller, fullerene, fulleride, STM

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