474. Title:Optical and vibrational properties of toroidal carbon nanotubes
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Abstract:Toroidal carbon nanotubes (TCNTs), which have been evaluated for their potential applications in terahertz communication systems, provide a challenge of some magnitude from a purely scientific perspective. A design approach to TCNTs, as well as a classification scheme, is presented based on the definition of the six hollow sections that comprise the TCNT, slicing each of them to produce a (possibly creased) planar entity, and projecting that entity onto a graphene lattice. As a consequence of this folding approach, it is necessary to introduce five- and seven-membered rings as defect sites to allow the fusing together of the six segments into final symmetric TCNTs. This analysis permits the definition of a number of TCNT geometry families containing from 108 carbons up to much larger entities. Based on density functional theory (DFT) calculations, the energies of these structural candidates have been investigated and compared with [60]fullerene. The structures with the larger tube diameters are computed to be more stable than C60, whereas the smaller diameter ones are less stable, but may still be within synthetic reach. Computational studies reveal that, on account of the stiffness of the structures, the vibrational frequencies of characteristic low-frequency modes decrease more slowly with increasing ring diameter than do the lowest optical excitation energies. It was found that this particular trend is true for the "breathing mode" vibrations when the diameter of the tubes is small, but not for more flexible toroidal nanotubes with larger diameters.