Bucky ball crystal revisited from a spectroscopic point of view

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Abstract : The determination of the structure complex crystal or molecular structures is always a challenging goal. As a test case, we have used C60 in bucky ball crystal (C60-crystal). The structure was previously determined by neutron scattering at liquid He temperature and Rietveld analysis by William et al. [1]. The crystal structure consist of a close packing of C60 with cubic symmetry.We have performed *ab initio* DFT-based phonon calculation using these coordinates. The phonon spectrum exhibits negative frequencies suggesting that the structure presents some instability. Thus the experimentally determined structure has been relaxed using density functional theory. High resolution electron energy loss spectroscopy at carbon K edge of bucky ball crystal has been recorded in a transmission electron microscope (TEM). The modeling of the spectrum in the Framework of GW-BSE with the OCEAN code show that it is best reproduced using the new "DFT-refined" coordinates.

[1] : William I. F. David, Richard M. Ibberson, Judy C. Matthewman, Kosmas Prassides, T. John S. Dennis, Jonathan P. Hare, Harold W. Kroto, Roger Taylor, and David R. M. Walton, Crystal structure and bonding of ordered C60, Nature **353** (1991), no. 6340, 147–149.