End spin formation in capped carbon nanotubes

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Abstract

Semiconducting open carbon nanotubes (CNTs) have been shown to exhibit topological bound states within the spectral gap [1], giving rise to spin formation at the ends of the nanotube [2]. However, the production of open-ended CNTs is difficult. Here, we investigate the electronic properties of capped topological CNTs using exact diagonalization and Chebyshev expansion methods to identify local resonances and bound states in the density of states at the end of long tubes [3]. While capping removes topological states, non-topological bound states and resonances localized on the pentagons appear, presumably related to Euler topology. We observe an abundance of local resonances and bound states, and about 20% of the investigated stable caps are predicted to produce end spins [4]. We identify a specific CNT of chirality (6,5) which produces well-defined end spins. This type of CNT can be produced with ultra-high purity (>95%) [5], and is an excellent candidate for a geometrically controlled spin qubit.

References

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Figures

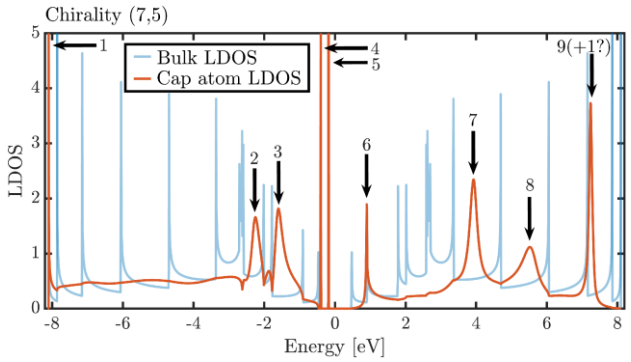

Figure 1: Characteristic resonances on a cap on the (7,5) chirality nanotube.

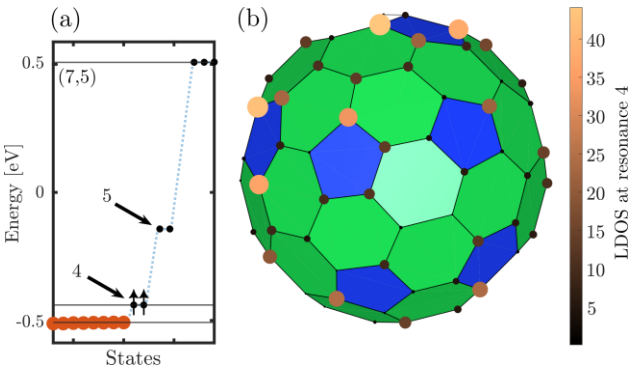

Figure 2: (a) Exact spectrum of the system near the gap. The lower energy degenerate bound state pair is half filled, giving rise to spin formation on the nanotube caps. (b) Spin localization on the nanotube cap. The spins preferentially occupy pentagons, indicating the importance of Euler topology.