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Jahn-Teller distortion of C(5,0) carbon nanotubes inside AlPO₄-5 zeolite channels MARIVI FERNANDEZ-SERRA, CECAM ENS-Lyon, Lyon, France, XAVIER BLASE, CNRS et LPMCN, universite Lyon 1, Lyon, France — The electronic structure of C(5,0) carbon nanotubes inside zeolite channels is studied by means of *ab initio* simulations. The band structure of the tubes is analyzed in detail as a function of the environment and the breaking of the LUMO state degeneracy and subsequent band-gap opening is interpreted as a Jahn-Teller distortion, previously refereed as Peierls instability, ocurrying at room temperature. However, we show that the zeolite matrix considerably screens this transition, reducing the opening of the gap observed in isolated tubes by more than 50%. A strong lateral interaction between the nanotube and the zeolite is revealed, but this is not enough to reconciliate the resulting picture of semiconducting tubes at T=300 K with the superconducting transition of CNTs inside AlPO₄-5 zeolite channels, observed at Tc=15 K.

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