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C60 Polymerization in BN and Carbon Nanopeapods ANDREA TRAVE[1], FILIPE J. RIBEIRO, STEVEN G. LOUIE, MARVIN H. COHEN, Dept. Physics, UC Berkeley & MSD, Lawrence Berkeley National Laboratory — A variety of C_{60} structures, polymerized and non-polymerized, isolated or encapsulated in BN or carbon nanotubes, have been analysed, to gain insight into the atomic and electronic structure of nanopeapods (NPP). Isolated double-bonded C_{60} chains and dimers are found to be more stable than non-polymerized C_{60}. NPP geometries and energetics are unaffected by encapsulation, which gives an energy gain larger than the activation energy for C_{60} polymerization, supporting the hypothesis of partial polymerization of C_{60} molecules in NPP's. Upon encapsulation, BN NPP's remain wide-gap semiconductors, while in metallic carbon NPP's the lowest unoccupied C_{60} states lie just above the Fermi level and charge transfert can take place, stabilizing single-bonded C_{60} chains with wider spacing than double-bonded polymers, closely corresponding to the experimental structural observations. This work was supported by NSF (Grant No.DMR-0087088), and by the Office of Energy Research, Office of Basic Energy Sources, Materials Sciences Division of the US Department of Energy (Contract No. DE-AC03-76SF00098). Part of this work was performed under the auspices of the US Department of Energy by the University of California at the LLNL (Contract No.W-7405-Eng-48). Computational resources at NERSC, NCSA, and NPACI are acknowledged.

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