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Investigation of $Gd_3N@C_{2n}$ ($40 \leq n \leq 44$) family by Raman and inelastic electron tunneling spectroscopy BRIAN BURKE, University of Virginia, JACK CHAN, KEITH WILLIAMS, JIECHAO GE, CHUNYING SHU, WUJUN FU, HARRY DORN, JAMES KUSHMERICK, ALEXANDER PURETZKY, DAVID GEOHEGAN, DEPARTMENT OF PHYSICS, UNIVERSITY OF VIRGINIA COLLABORATION, DEPARTMENT OF CHEMISTRY, VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY COLLABORATION, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION, CENTER FOR NANOPHASE MATERIALS SCIENCES, OAK RIDGE NATIONAL LABORATORY COLLABORATION — The structure and vibrational spectrum of $Gd_3N@C_{80}$ is studied through Raman and inelastic electron tunneling spectroscopy (IETS) as well as density functional theory (DFT) and universal force field (UFF) calculations. Hindered rotations, shown by both theory and experiment, indicate the formation of a $Gd_3N{-}C_{80}$ bond which reduces the ideal icosahedral symmetry of the C_{80} cage. The vibrational modes involving the movement of the encapsulated species are a fingerprint of the interaction between the fullerene cage and the core complex. We present Raman data for the $Gd_3N@C_{2n}$ ($40 \leq n \leq 44$) family as well as $Y_3N@C_{80}$, $Lu_3N@C_{80}$, and $Y_3N@C_{88}$ for comparison. Conductance measurements have been performed on $Gd_3N@C_{80}$ and reveal a Kondo effect similar to that observed in C_{60}.

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