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Structural and magnetic properties of $Tc_n@C_{60}$ endohedral metallofullerenes: An *ab initio* study[1] EUNJA KIM, PHILIPPE F. WECK, KENNETH R. CZERWINSKI, University of Nevada Las Vegas, DAVID TOMÁNEK, Michigan State University — We use *ab initio* spin density functional calculations to study the equilibrium structure and magnetic properties of $Tc_n@C_{60}$ endohedral metallofullerenes. The radionuclide ^{99m}Tc is well established in biomedicine as a potent *in vivo* diagnostic radiopharmaceutical; its encapsulation in the inert C_{60} shell is expected to limit possible cytotoxicity of radiometal nanoparticles catabolized by the biological host. We find that C_{60} can endohedrally accommodate Tc_n clusters with up to $n = 7$. The encapsulation does not change significantly the structure of the enclosed clusters, but reduces the magnetic moment due to a stronger Tc–C hybridization for the larger clusters.

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