Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Endohedral fullerenes contaning transition-metal clusters[1]
SHUSIL BHUSAL, LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We report detailed investigation of structural, electronic, and spectroscopic properties of VSc_2N-containing fullerenes in the size range C_{68} - C_{96}. First, the candidate structures of the ground state are obtained using a systematic approach in which a large number of isomers of endohedral fullerenes were screened for their energetic stability. Stability of some of the most promising isomers were further studied using density functional theory at the all-electron level using large polarized Gaussian basis sets. The effect of the V doping is examined on the structure, spin states and the magnetic properties of the endohedral fullerenes.

[1]De-SC0002168, NSF-DMR 125302, DE-SC0006818

Tunna Baruah
University of Texas at El Paso

Date submitted: 11 Nov 2016 Electronic form version 1.4