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Electronic and optical properties of VSc2N@C68 fullerene SHUSIL BHUSAL, University of Texas at El Paso — We report a detailed investigation on structural, electronic, and spectroscopic properties of the VSc2N@C68. The candidate structures for the ground state are obtained using a systematic approach. Our results indicate that the isomer 6079 of C68 yields the lowest energy structure of VSc2N@C68 at DFT level. The doping by V leads to an overall spin magnetic moment of 1 muB for the cluster. The ionization energy, electron affinity, the quasi-particle gap, and vibrational analysis of the lowest energy isomer indicate a stable molecule. The calculated infrared, Raman and optical spectra of the most stable fullerene can help in experimental identification.

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