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The Study of Hypothetical Carbon Allotropes Using Hartree Fock and Density Functional Computational Methods P.A. ECTON, C.J. MORRIS, J.M. PEREZ, Department of Physics, University of North Texas, S.G. SRIVILLIPUTHUR, Department of Materials Science and Engineering, University of North Texas, G.F. VERBECK, Department of Chemistry, University of North Texas — We have investigated the possibility of hypothetical alternative carbon allotropes using computational methodologies using Gaussian and VASP molecular simulation programs. We investigate the possible existence of carbon based balls, nanotubes and sheets composed of hexagonal rings, cyclobutane rings or pentagonal rings. The possibility of the existence of a hypothetical allotrope is determined by the convergence of the given allotrope under geometric optimization. The theories used to compute such convergence are Hartree-Fock theory and density functional theory. The theoretical Raman spectra of each allotrope can also be computed using Gaussian. The results concerning the reality of the substances under investigation are inconclusive except for a C_{24} ball, which has been shown to converge to graphene and is therefore an unstable molecule.

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