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Theoretical Investigation of the Vibrational and Electronic Properties of Titanium Carbide Nanocrystals QIN ZHANG, STEVEN LEWIS, The University of Georgia — Stable titanium carbide nanoclusters with ˜1:1 stoichiometry were first discovered in molecular-beam experiments in the early 1990's. These clusters are all indexed to perfect or nearly perfect $N_1 \times N_2 \times N_3$ fragments of bulk TiC in the rocksalt structure and are thus termed "nanocrystals". The most abundant member of this family is the $3 \times 3 \times 3$ nanocrystal $Ti_{14}C_{13}$, indicating special stability for this species. Using Density Functional Theory, we have carried out a detailed theoretical analysis of the structural, electronic, and vibrational states of $Ti_{14}C_{13}$ and its $3 \times 3 \times 3$ sibling, $Ti_{13}C_{14}$, which is not observed in the experiments. In this talk, we will present our theoretical results and show how our analysis sheds light on several previously unresolved experimental findings.

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