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Structure and Stability of Metal Oxide Nanowires DE NYAGO TAFEN, JAMES LEWIS, West Virginia University, Morgantown, WV — We present a comprehensive theoretical study — within the framework of *ab initio* density functional theory method — of the structural and stability properties of metal oxide nanowires. We consider nanowires with $\langle 100 \rangle$ growth direction with several diameters and surface facet configurations. A stability analysis of the results obtained for theses nanowires is used to determine the most stable geometries. We show that the perimeter of the nanowires is a meaningful dimensional parameter, and that the surface facets play a central role on the energetics of the nanowires. The results are compared to available experimental data.

De Nyago Tafen
West Virginia University, Morgantown, WV

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