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A Calculation of the Electronic Structure of Gallium Phosphide Nanotubes PETER LYON[1], BRET HESS[2], Brigham Young University, BYU CONDENSED MATTER PHYSICS TEAM — We studied the band structure and density of states of both zigzag and armchair gallium phosphide nanotubes using density functional theory with a quantum chemistry program called VASP. We were able to show that all gallium phosphide nanotubes are narrow band-gap semiconductors. We have also shown that all zigzag nanotubes have indirect band gaps and that all armchair nanotubes have direct band gaps. Furthermore, we calculated that increasing the radius of armchair nanotubes led to a decrease in the band gap but that there was no similar change in the band gap of zigzag nanotubes as radius increased.

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