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Investigation of the changes in the density of states in the Copper-Titanium system[1] A. CHOURASIA, Texas A&M University-Commerce — The density of states and structure parameters in the copper-titanium system have been investigated by DFT. Various compounds of the copper and titanium (such as CuTi, CuTi2, CuTi3, Cu3Ti) have been studied. The DFT calculations were performed using the GGA exchange-correlation potential. For each compound the atoms were relaxed by minimizing the forces and allowing changes in the unit cell. Geometrical structure and variations in the density of states in the vicinity of the Fermi level have correlated with the near neighbors of copper/titanium.

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