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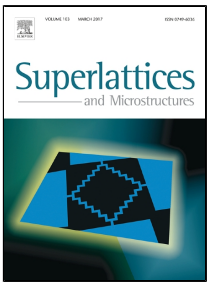

Structural, Electronic, Mechanical and Quantum Transport of Ultrathin Gold Nanowire: A Density Functional Approach

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Highlights:

- We have investigated gold (Au) nanowires having different cross-section with 1–10 Au atoms per unit cell by using first-principles calculations based on density-functional theory.
- The electronic band structures of different structure which represents that all the nanowires are metallic in nature.
- The numbers of conductional channel are determined from the electronic band structures.
- The number of conduction channels inflates when the nanowire becomes thicker with increasing number of atoms per unit cell.