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# Electronic and Mechanical Material Properties from DFT Calculations

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## ABSTRACT

Materials modeling provides a cost and time efficient method for studying their properties, especially in nanotechnology where length and time scales are not accessible experimentally. Our research focuses on developing a tool useful for both instructional and research purposes that calculates material properties. The tool relies on density functional theory (DFT) calculations to compute specific properties for a wide range of materials including semiconductors, insulators, and metals. A major goal with our tool was to keep the GUI very simple for novice users, such as students, while retaining an advanced option section for experienced users, such as researchers. The tool can compute electronic band structures, density of states, bulk modulus, dielectric constants and other properties of the material. Furthermore, the user can select from various pre-set materials or create one of their own by specifying the atomic structure. The end-product we have built combines the simplicity of a teaching tool with the versatility of a research tool, resulting in a powerful simulation package.

## KEYWORDS

DFT, simulation, materials science, material properties, nanotechnology