



DENSITY FUNCTIONAL THEORY AS A MAJOR TOOL IN COMPUTATIONAL MATERIALS SCIENCE

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INTRODUCTION

It is now widely recognized that atomistic simulations—especially those employing density functional theory—are becoming an increasingly important part of materials science today. However, a great variety of approaches and implementations have been developed that make the situation confusing not only to the non-expert, but perhaps even to the specialist. For this reason, we describe here the local density formulation of density functional theory in enough detail to provide some understanding of this now fairly well-developed, important, and most successful approach for studying electronic structure phenomena in materials.

It should be borne in mind that the fundamental atomistic principles underlying the structural and functional behavior of materials are astonishingly simple: (*a*) For most purposes, atomic nuclei can be treated as classical particles with a given mass and positive charge; (*b*) electrons are particles of spin one half, thus obeying the Pauli exclusion principle; their kinetic behavior is described by quantum mechanics; and (*c*) the only relevant interactions are of an electrodynamic nature, in particular, attrac-

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