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Density functional theory (DFT) is by now a well-established method for tackling the quantum mechanics of many-body systems. Originally applied to compute properties of atoms and simple molecules, DFT has quickly become a work horse for more complex applications in the chemical and materials sciences.

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Walter Kohn indeed gave a major impulse to the dissemination of density functional theory in physics and chemistry (several applications in biology andgeologyhavealsoappeared!),butinordertohave“chemicalaccuracy” furtherstepshavetobetaken. It is the task of the new generation to continue the past and present e?ortsinthisexciting?eld.Wehopewiththis“primer”indensityfunctional ...

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choiceoftheword “theory”isunfortunate. It seemstoimply thatoneis free It seemstoimply thatoneis free to invent the way the world is constituted, or that physics is just one way to

graphs on the variants and applications of density functional theory exist, the aim of these lecture notes is to provide a careful introduction into the safe basis of this type of theory for both beginners and those working in

Density-Matrix Renormalization: A New Numerical Method in Physics Lectures of a Seminar and Workshop Held at the Max-Planck-Institut für Physik komplexer Systeme Dresden, Germany,August 24th to September 18th, 1998

Abstract. This chapter introduces thermal density functional theory, starting from the ground-state theory and assuming a background in quantum mechanics and statistical mechanics.

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