<<基础电子结构>>

图书基本信息

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作者：Walter A.Harrison

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内容概要

This text presents an account of analytic electronic structure, to be distinguished from computational electronic structure. Both are based upon a one-electron approximation, local-density theory, and the determination of the quantum-mechanical electronic states. They both seek to predict the properties of the resulting solids, or molecules on the basis of these states. In the computational mode, the minimum number of approximations are used, and numerical solutions are sought. Here we seek instead to focus on the most important aspects of the solution, making what approximations are necessary in order to proceed analytically and obtain formulae for the properties. This reducing of the problem to basics is almost always less accurate that the computational solution, but has the advantage that it displays the dependence of any property on the parameters Of the system. It gives us an understanding of the property in a sense that a numerical solution, or a direct measurement, cannot.

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