

A detailed ball-and-stick molecular model of a polymer chain, likely polyethylene, is shown against a blue background. The model features a long, zigzag backbone of carbon atoms (grey) and hydrogen atoms (white). Red spheres represent oxygen atoms, and a few blue spheres represent nitrogen atoms, suggesting a more complex polymer or a specific functional group. The model is oriented diagonally across the frame.

# DENSITY FUNCTIONAL THEORY

A PRACTICAL INTRODUCTION

*David S. Sholl    Janice A. Steckel*

 WILEY

# Density Functional Theory A Practical Introduction

**Carsten A. Ullrich**



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