

# CONTENTS

Preface	vii
<i>Ab-Initio</i> Molecular Dynamics Simulation of Structural Phase Transitions <i>P. Focher and G. L. Chiarotti</i>	1
Boson Many-Body Problem: Progress in Variational Monte Carlo Computations <i>L. Reatto</i>	43
Monte Carlo Variational Theory for Fermions <i>M. H. Kalos and L. Reatto</i>	99
Recent Developments of Device Simulation Tools for Parallel Processing <i>M. Saraniti and P. Lugli</i>	114
Simulation of Classical and Quantum Activated Processes in the Condensed Phase <i>G. Ciccotti, M. Ferrario, D. Laria and R. Kapral</i>	150
' <i>Ab-Initio</i> ' Calculations of Electronic Properties of Metallic Solid Solutions <i>E. Bruno, P. Donato, G. Florio, B. Ginatempo and E. S. Giuliano</i>	191
<i>Ab-Initio</i> Calculation of the Electronic (Valence and Core) and Optical Properties of Interfaces <i>S. Ossicini and O. Bisi</i>	238