

CONTENTS

Preface	v
1. Molecular Electronics with Gaussian98/03 <i>J. J. Palacios, A. J. Pérez-Jiménez, E. Louis, E. SanFabián, J. A. Vergés and Y. García</i>	1
2. Molecular Dynamics Simulations of Single Molecule Atomic Force Microscope Experiments <i>W. Nowak and P. E. Marszalek</i>	47
3. Molecular Dynamics Simulations of a Molecular Electronics Device: The NanoCell <i>J. Seminario, P. Derosa, L. Cordova and B. Bozard</i>	85
4. Computation of Excited State Potential Energy Surfaces via Linear Response Theories Based on State Specific Multi-Reference Coupled Electron-Pair Approximation Like Methods <i>S. Chattopadhyay, D. Pahari, U. Mahapatra, D. Mukherjee</i>	121
5. Modelling of Anisotropic Exchange Coupling in Rare-Earth-Transition-Metal Pairs: Applications to $\text{Yb}^{3+}\text{-Mn}^{2+}$ and $\text{Yb}^{3+}\text{-Cr}^{3+}$ Halide Clusters and Implications to the Light Up-Conversion <i>M. Atanasov, C. Daul and H. U. Güdel</i>	153
6. Is a Dihydrogen Bond a Unique Phenomenon? <i>S. J. Grabowski and J. Leszczynski</i>	195
Index	237
Content Index	243