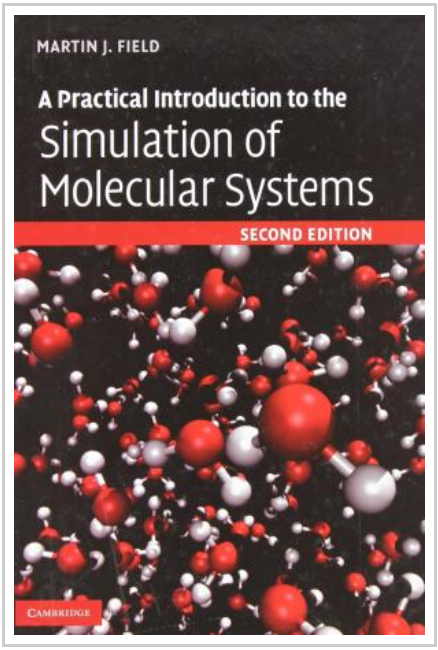

A practical introduction to the simulation of molecular systems

By -

2015. Soft cover. Book Condition: New. 1st Edition. Preface to the first editionPreface to the second edition1 Preliminaries1.1 Introduction1.2 Python1.3 Object-oriented programming1.4 The pDynamo library1.5 Notatioand units2 Chemical models and representations2.1 Introduction2.2 The System class2.3 Example 12.4 Commomolecular representations2.5 Example 23 Coordinates and coordinate manipulations3.1 Introduction3.2 Connectivity3.3 Internal coordinates3.4 Example 33.5 Miscellaneous transformations3.6 Superimposing structures3.7 Example 44 Quantum chemical models4.1 Introduction4.2 The Born-Oppenheimer approximation4.3 Strategies for obtaining energies oa potential energy surface4.4 Molecular orbital methods4.5 The Hartree-Fock approximation4.6 Analysis of the charge density4.7 Example 54.8 Derivatives of the potential energy4.9 Example 65 Molecular mechanics5.1 Introduction5.2 Typical empirical energy functions5.3 Calculating a molecular mechanics energy5.4 Example 75.5 Parametrizing potential energy functions5.6 Soft constraintsHybrid potentials6.1 Introduction6.2 Combining QC and MM potentials6.3 Example 86.4 Covalent bonds betweeQC and MM atoms6.5 Example 9Finding stationary points and reactiopaths opotentialenergy surfaces7.1 Introduction7.2 Exploring potential energy surfaces7.3 Locating minima7.4 Example 107.5 Locating saddle points7.6 Example 117.7 Following reactiopaths7.8 Example 127.9 Determining complete reactiopaths7.10 Example 138 Normal mode analysis8.1 Introduction8.2 Calculatioof the normal modes8.3 Rotational and translational modes8.4

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