

Introduction to Computational Chemistry

Frank Jensen



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Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics:

- * Polarizable force fields
- * Tight-binding DFT
- * More extensive DFT functionals, excited states and time dependent molecular properties
- * Accelerated Molecular Dynamics methods
- * Tensor decomposition methods
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