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Density functional theory - Wikipedia

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Computational chemistry - Wikipedia
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Between them, one can consider: root finding
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Computational physics - Wikipedia

Finally Chapter 5 applies these methods to problems of contemporary interest. The book is designed to be a junior/senior level text in computational quantum mechanics, suitable for undergraduates and graduates in chemistry, physics, computer science, and associated disciplines. Contents:
Formulations of Quantum Mechanics

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These include LCAO, Hartree-Fock-SCF method for molecules, Roothaan LCAO-MO-SCF method, and electron correlation energy. Chapter 4 is devoted to the more sophisticated computational methods in quantum chemistry, with an introduction to topics that include:

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the zero differential overlap approximation;
Huckel MO theory of conjugated molecules;
Pariser-Parr-Pople MO method; extended Huckel
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CNDO; INDO; NDDO; MINDO ...

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Quantum ...

Good knowledge in molecular quantum
mechanics, statistical mechanics and
molecular simulation methods is expected.
First-hand experience with non-adiabatic

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molecular dynamics simulation techniques (e.g. fewest switches surface hopping or Ehrenfest) is an advantage but not required.

Research Fellow in Computational
Physics/Chemistry at UCL

Computational Methods in Physics, Chemistry and Biology offers an accessible introduction to key computational techniques used within science, including quantum mechanics, dynamics, evolutionary methods and molecular dynamics.

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Joel Franklin, Computational Methods for
Physics, Cambridge University Press (2013).

Alejandro L. Garcia, Numerical Methods for
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(2000). Richard J. Gaylord and Paul R.

Wellin, Computer Simulations with
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