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Density functional theory - Wikipedia

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Computational chemistry - Wikipedia

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Computational physics - Wikipedia

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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: the zero differential overlap approximation; Huckel MO theory of conjugated molecules; Pariser-Parr-Pople MO method; extended Huckel theory; neglect of differential overlap methods; invariance in space requirements; CNDO; INDO; NDDO; MINDO ...

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

Computational Methods in Physics, Chemistry and Biology ...

Joel Franklin, Computational Methods for Physics, Cambridge University Press (2013). Alejandro L. Garcia, Numerical Methods for Physics, second edition, Prentice Hall (2000). Richard J. Gaylord and Paul R. Wellin, Computer Simulations with Mathematica: Explorations in Complex Physical and Biological Systems, Springer-Verlag (1995).

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