
**Título:** Essentials Of Computational Chemistry. Theories And Models

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**Sinopsis**

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Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.

Essentials of Computational Chemistry, Theories and Models, Second Edition provides an accessible introduction to this fast developing subject. Extensively revised and updated, the Second Edition has been carefully developed to encourage student understanding and to establish seamless

connections with the primary literature for the advanced reader. The book opens with a presentation of classical models, before gradually moving on to increasingly more complex quantum mechanical and dynamical theories. Coverage and examples are drawn from inorganic, organic and biological chemistry.

evolving topics like density functional theory, continuum solvation models, and computational thermochemistry brought firmly up-to-date

carefully guides the reader through key equations, providing background information and placing each in context.

numerous examples and applications with selected case studies designed as a basis for classroom discussion.

supplementary website with exercises problems and updates: www.pollux.chem.umn.edu/8021/

Invaluable to all students taking a first course in computational chemistry, molecular modelling, computational quantum chemistry or electronic structure theory. This book will also be of interest to postgraduates, researchers and professionals needing an up-to-date, accessible introduction to this subject.