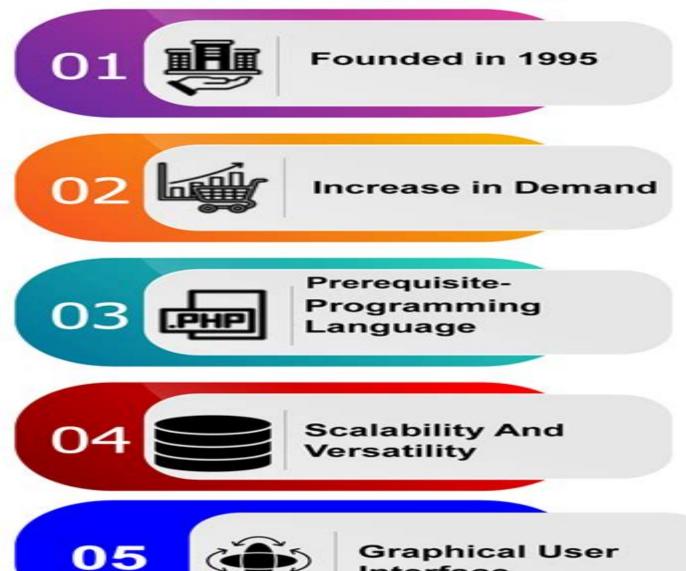


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Handbook of Computational Chemistry Jerzy Leszczynski, 2012-01-13 The role the Handbook of Computational Chemistry is threefold It is primarily intended to be used as a guide that navigates the user through the plethora of computational methods currently in use it explains their limitations and advantages and it provides various examples of their important and varied applications This reference work is presented in three volumes Volume I introduces the different methods used in computational chemistry Basic assumptions common to the majority of computational methods based on molecular quantum or statistical mechanics are outlined and special attention is paid to the limits of their applicability Volume II portrays the applications of computational methods to model systems and discusses in detail molecular structures the modelling of various properties of molecules and chemical reactions Both ground and excited states properties are covered in the gas phase as well as in solution This volume also describes Nanomaterials and covers topics such as clusters periodic and nano systems Special emphasis is placed on the environmental effects of nanostructures Volume III is devoted to the important class of Biomolecules Useful models of biological systems considered by computational chemists are provided and RNA DNA and proteins are discussed in detail This volume presents examples of calcualtions of their properties and interactions and reveals the role of solvents in biologically important reactions as well as the structure function relationship of various classes of Biomolecules A Chemist's Guide to Valence Bond Theory Sason S. Shaik, Philippe C. Hiberty, 2007-12-10 This reference on current VB theory and applications presents a practical system that can be applied to a variety of chemical problems in a uniform manner After explaining basic VB theory it discusses VB applications to bonding problems aromaticity and antiaromaticity the dioxygen molecule polyradicals excited states organic reactions inorganic organometallic reactions photochemical reactions and catalytic reactions With a guide for performing VB calculations exercises and answers and numerous solved problems this is the premier reference for practitioners and upper level students The Module and Programme Development Handbook Jennifer Moon, 2003-12-16 This book shows how to design and develop educational programmes that are linked logical and successful with clear step by step guidance on the processes involved It shows how to develop courses that successfully meet quality and assessment criteria including those set by the Quality Assurance Agency and provides a route map through the various elements involved The author shows how to design modules with clearly defined levels for assessment outcomes and quality criteria and which meet standard teaching and learning expectations Developed to be accessible straightforward systematic and practical it is illustrated throughout with examples and concise summaries Key features include clear simple guidance on developing a module understanding levels and level descriptors setting aims and learning outcomes developing assessment methods and criteria devising teaching strategies staff development activities guidance on programme specification **Introducing the IB Diploma Programme** Marc Abrioux, Jill Rutherford, 2013-02-14 Schools wishing to introduce the IB diploma programme are faced with major investment

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