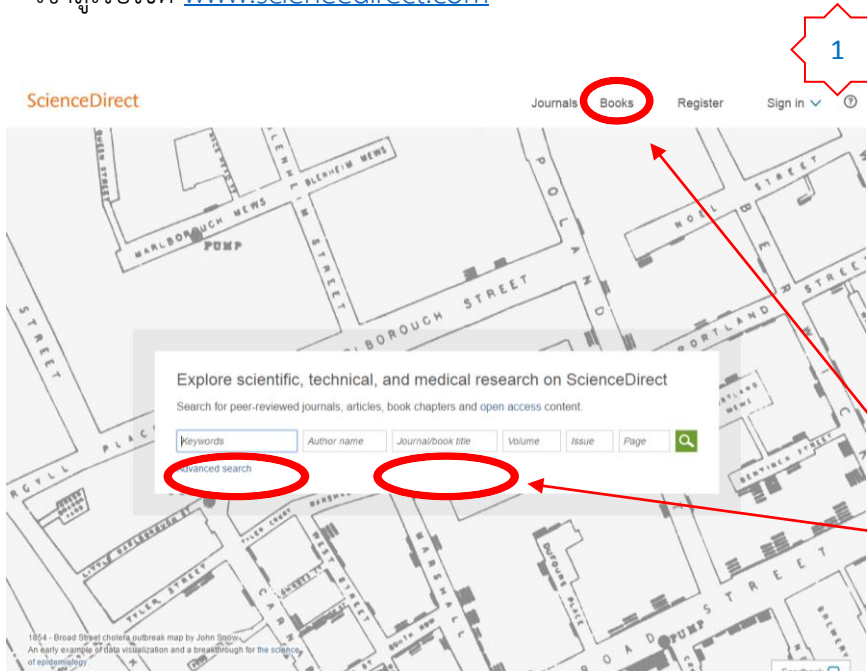


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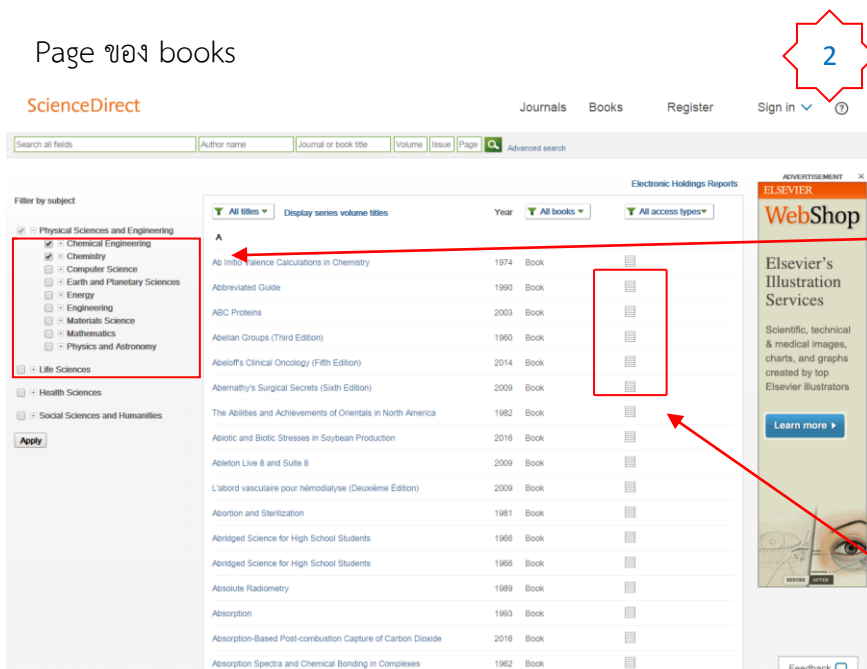
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Ab Initio Valence Calculations in Chemistry describes the theory and practice of ab initio valence calculations in chemistry and applies the ideas to a specific example, linear BEH2. Topics covered include the Schrödinger equation and the orbital approximation to atomic orbitals; molecular orbital and valence bond methods; practical molecular wave functions; and molecular integrals. Open shell systems, molecular symmetry, and localized descriptions of electronic structure are also discussed. This book is comprised of 13 chapters and begins by introducing the reader to the use of the Schrödinger equation to solve the electronic structure of molecular systems. This discussion is followed by two chapters that describe the chemical and mathematical nature of orbital theories in quantum chemistry. Two general ways of using chemical and physical information in looking for approximate solutions of the Schrödinger equation are highlighted: model approximations and numerical approximations. Attention then turns to atomic orbitals as the basis of a description of molecular electronic structure; practical molecular wave functions; and a general strategy for performing molecular valence calculations. The final chapter examines the nature of the valence electronic structure by using invariance with respect to transformations among the occupied molecular orbitals and among the atomic orbitals. This text will be of interest to students.

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Ab Initio Valence Calculations in Chemistry describes the theory and practice of ab initio valence calculations in chemistry and applies the principles to several specific topics covered include the Schrödinger equation and the orbital approximation to atomic orbitals, molecular orbital and valence bond methods, practical molecular wave functions, and molecular integrals. Open shell systems, molecular symmetry, and localized descriptions of electronic structure are also discussed.

This book is comprised of 13 chapters and begins by introducing the reader to the use of the Schrödinger equation to solve the electronic structure of molecular systems. This discussion is followed by two chapters that describe the chemical and mathematical nature of orbital theories in quantum chemistry. Two general ways of using chemical and physical information in looking for approximate solutions of the Schrödinger equation are highlighted: model approximations and numerical approximations. Attention then turns to atomic orbitals as the basis of a description of molecular electronic structure, practical molecular wave functions, and a general strategy for performing molecular valence calculations. The final chapter examines the nature of the valence electronic structure by using invariance with respect to transformations among the occupied molecular orbitals and among the atomic orbitals.

This text will be of interest to students of chemistry and physicists.

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