

What is Ab Initio

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Founded in 1995

02



Increase in Demand

03



**Prerequisite-
Programming
Language**

04



**Scalability And
Versatility**

05



**Graphical User
Interface**

Ab Initio Program Guide

Sason S. Shaik, Philippe C. Hiberty



Ab Initio Program Guide:

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and advantages and providing examples of their applications The first part outlines methods the balance of volumes present numerous important applications

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A Chemist's Guide to Valence Bond Theory Sason S. Shaik,Philippe C. Hiberty,2007-12-04 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

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