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Goal of this Presentation

General physical  
background

(understanding what  
goes into calculation)

Understanding which  
parameter exist and  
what they do (aimed at  
Gaussian)

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The term computational

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chemistry is usually  
used when a  
mathematical method is  
sufficiently well  
developed that it can be  
automated for  
implementation on a  
computer. Note that the  
words exact and perfect  
do not appear in these  
definitions.

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models although the  
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chemistry is a branch of



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chemistry that uses computer simulation to assist in solving complex chemical problems. It exploits methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures, the interactions, and the properties of molecules.

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Chemistry, [10.1002/jcc.26126](https://doi.org/10.1002/jcc.26126), 41,  
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Wojtek Gren April 16,

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Preface Before

beginning please note

that as many terms used

are either unique to

computational chemistry

or have a unique

meaning in this context

a glossary of these

terms, which will appear

in bold face is given at

the end. Also the ...

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Chemistry provides a comprehensive account of the fundamental principles underlying different methods, ranging from classical to sophisticated quantum models.

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| Frank Jensen ...

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chemistry is also used to

study the fundamental

properties of atoms,

molecules, and chemical

reactions, using

quantum mechanics and

thermodynamics.

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use mathematical

algorithms, statistics,

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with experimental  
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