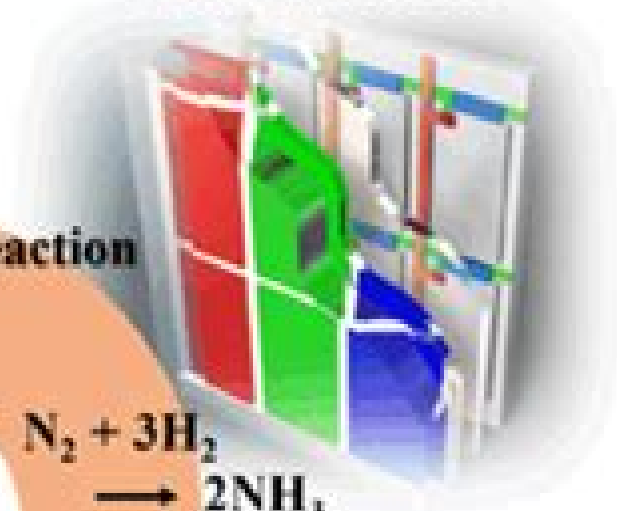


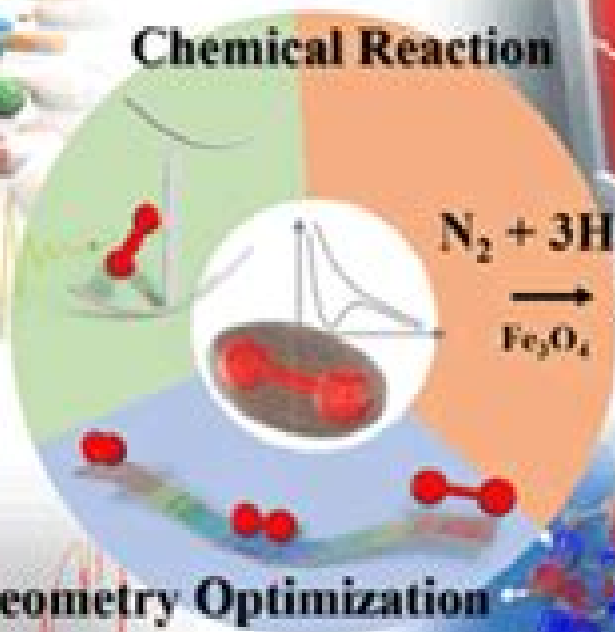
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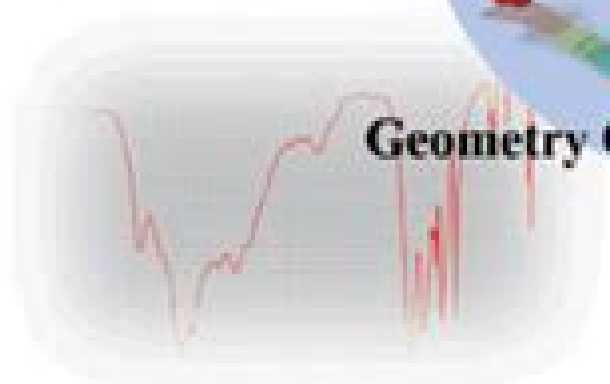
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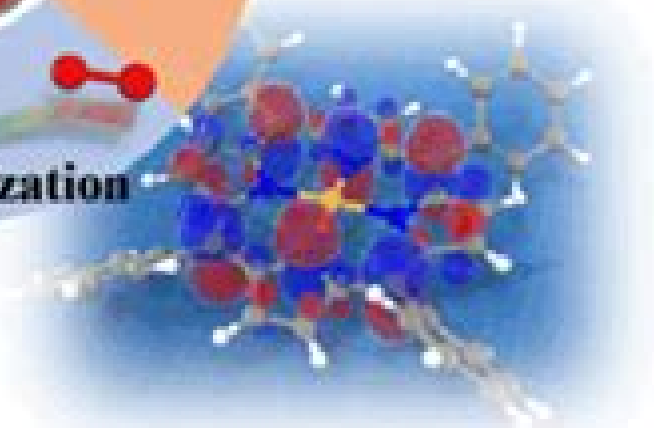
Chemical Reaction



Geometry Optimization



Molecular spectroscopy



Complex molecular dynamics

Figure 1: Applications of computational chemistry.

Computer Software Applications In Chemistry

Ashish Kumar

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Computers and Their Applications to Chemistry Ramesh Kumari,2005 Introduces the fundamentals of BASIC FORTRAN and C language using the concepts of Chemistry This book includes an account of various statements input output format control if then else go to do loops and more has been illustrated by various examples

Computer Software Applications in Chemistry Peter C. Jurs,1986-11-05 This unique presentation of computer software applications in chemistry goes beyond hardware interfacing and computer lab use The book is organized by topic general aspects of computers solution of equations by numerical means abstract nonnumerical chemical structure information handling and molecular mechanics and graphical displays of data and molecular structures Each topic is supplemented frequently by FORTRAN programs which illustrate the ways in which computer software is applicable to the chemical field

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