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Ab initio quantum chemistry methods are computational chemistry methods based on quantum chemistry. The term ab initio was first used in quantum chemistry by Robert Parr and coworkers, including David Craig in a semiempirical study on the excited states of benzene. The background is described by Parr. Ab initio means "from first principles" or "from the beginning", implying that the only ...

### **Ab initio quantum chemistry methods - Wikipedia**

Language ab initio SL. If a student has no previous background in a given language, then that student may study that language as an ab initio SL subject. Such a course focuses on giving the student basic knowledge of both the language in everyday use and the culture of the places where it is spoken.

### **IB Group 2 subjects - Wikipedia**

Information for prospective undergraduate students at the Department of Language and Linguistic Science at the University of York.

### **Department of Language and Linguistic Science**

5 Grading Due to Alberta Education's requirements, students will receive both a IB grade, determined solely by the I's external assessments and internal assessments, as well as a "regular" Alberta grade, which

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Graphite and Hexagonal Boron-Nitride Possess the Same Interlayer Distance. Why? Oded Hod School of Chemistry, The Sackler Faculty of Exact Sciences, Tel Aviv

### **Graphite and Hexagonal Boron-Nitride Possess the Same**

arXiv:0904.4793v1 [physics.chem-ph] 30 Apr 2009 Henry's Law Constants of Methane, Nitrogen, Oxygen and Carbon Dioxide in Ethanol from 273 to 498 K:

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Ring-Puckering Motion of Azetidinium Cations in a Metal-Organic Perovskite  $[(CH_2)_3NH_2][M(HCOO)_3]$  (M = Zn, Mg) A Thermal and  $^1H$  NMR Relaxation Study

### **The Journal of Physical Chemistry C (ACS Publications)**

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Ming, Pingbing Position: Professor at Lsec, Institute of Computational Mathematics and Scientific/Engineering Computing, AMSS, Chinese Academy of Sciences Address: No. 55, East Road Zhong-Guan-Cun, Beijing, 100190, China Office: Room 726, South Building of AMSS

### Home page of Pingbing Ming - c c

Feasibility Studies. For those interested in determining if Vibrational Circular Dichroism (VCD) analysis is appropriate to their applications or specific chiral molecules, BioTools offers feasibility studies using the ChirallRâ,,ç instrument.

### BioTools - Chirality & Biologics

The Born-Oppenheimer Approximation C. David Sherrill School of Chemistry and Biochemistry Georgia Institute of Technology March 2005 We may write the nonrelativistic Hamiltonian for a molecule as a sum of  $\hat{h}_i$  terms:

### The Born-Oppenheimer Approximation

2 consider the electric field far away from the dipole moment. Taylor's series is used to study this behavior.  $E = kq(x^2/r^3)2kq(x+r)^2(10)$  An electric field further away from the dipole is obtained

### Applications of Taylor Series - University of Tennessee

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### Nicolas Onofrio - Google Scholar Citations

Vibrational excitation of Hz 0 by electrons 1997 ab initio target wavefunction. The effects of electron exchange and target polarization are approximately taken into account through the model potentials,  $V_{ex}$  and  $V_p$ , respectively. For  $V_c$ , use is made of the Hara version of the free electron gas model (Hara 1967). For  $V_p$ , we take the parameter-free correlation-polarization model of Padial and ...

### Electron-impact vibrational excitation of water molecules

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The scorpion is a cartoon analogue of the chelating ligand H<sub>2</sub>hox. It has claws (chÄ“lÄ“, in Greek), from which the word chelation is derived, and it shows beautiful fluorescence under UV light (as does the [Ga(hox)]<sup>+</sup> cation). The race shows that H<sub>2</sub>hox has faster kinetics to chelate the 68 Ga<sup>3+</sup> ion, the trophy in

this race, compared with the macrocyclic chelator H 4 DOTA (the slower crab).

### **Inorganic Chemistry (ACS Publications)**

Steven G. Louie received his Ph.D. in physics from UC Berkeley in 1976. After having worked at the IBM Watson Research Center, Bell Laboratories, and University of Pennsylvania, he joined the UC Berkeley faculty in 1980.

### **Steven Louie | UC Berkeley Physics**

1 Can We Estimate the Accuracy of ADMET Predictions? Igor V. Tetko,1,2,\* Pierre Bruneau,3 Hans-Werner Mewes,1 Douglas C. Rohrer,4 Gennadiy I. Poda4 1 " GSF - Institute for Bioinformatics, 85764 Neuherberg, Germany

### **Igor V. Tetko,1,2,\* Pierre Bruneau, Hans-Werner Mewes**

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### **GAUSSIAN 09W TUTORIAL - McGill University**

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### **List of New Projects Sanctioned under Women Scientists**

Advances in Colloid and Interface Science 93 2001 135½. 224 Adsorption from theory to practice A. Dańbrowski Faculty of Chemistry, M.Curie-Skłodowska University, 20031 Lublin, Poland

### **Adsorption from theory to practice - Indian Institute of**

Source: Encyclopedia of Library and Information Science, Ed. by Allen Kent and others, Vol. 25, 1978, published by Marcel Dekker Inc., New York. S.R. Ranganathan - A Short Biography BIRTH AND PARENTAGE ACTIVITIES AT MADRAS FAMILY LIFE ACTIVITIES AT BANARAS

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No specific proposals for attaching tooltip molecules such as the one illustrated in Figure 2 A/B to larger tool handles, or complete tools for positional diamond mechanosynthesis, have previously been reported in the scientific, engineering or patent literature. While others have previously noted the need for a handle structure to manipulate the active mechanosynthetic tooltip [32, 33, 36, 38 ...

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