MATERIALS SCIENCE & ENGINEERING
TEXAS A&M UNIVERSITY

Introduction to Materials Science & Engineering

Quantum Mechanics

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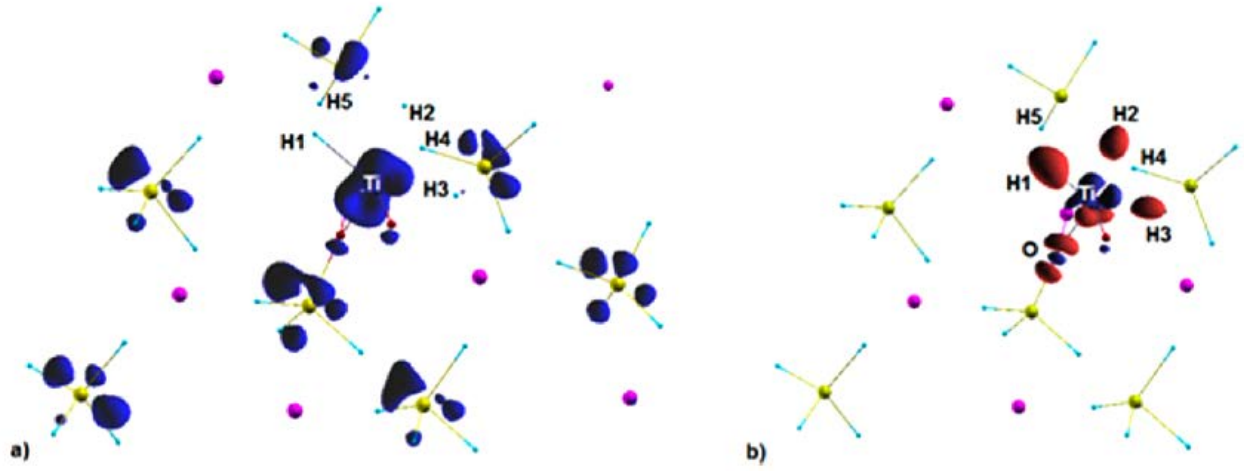
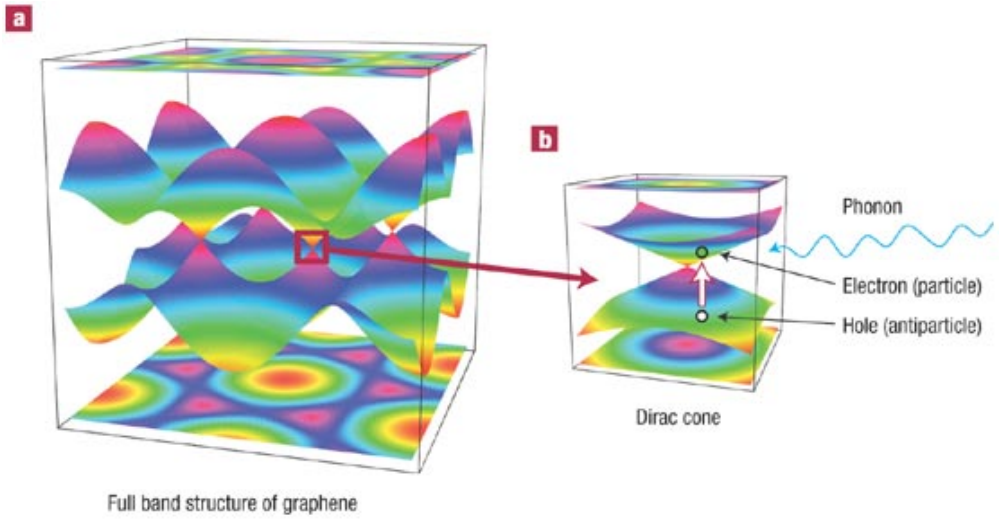


Effects of Titanium-Containing Additives on the Dehydrogenation Properties of $LiAlH_4$: A Computational and Experimental Study

Jennifer L. Wohlwend,[*,†,‡] Placidus B. Amama,[†,§] Patrick J. Shamberger,[†] Vikas Varshney,[†,‡] Ajit K. Roy,[†] and Timothy S. Fisher[†,⊥]



Nature Materials 6, 176 - 177 (2007), doi:10.1038/nmat1851
Graphene: Phonons behaving badly, Antonio H. Castro Neto[1]

Time Independent Schroedinger Equation:

$$E\Psi = \hat{H}\Psi$$

$$E\Psi(\mathbf{r}) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r})$$

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Solution to the Hydrogen Atom:

$$\psi_{n\ell m}(r,\theta,\phi) = \sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-\ell-1)!}{2n[(n+\ell)!]}}e^{-r/na_0}\left(\frac{2r}{na_0}\right)^{\ell}L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)\cdot Y_{\ell}^{m}(\theta,\phi)$$

Quantum Numbers: rules

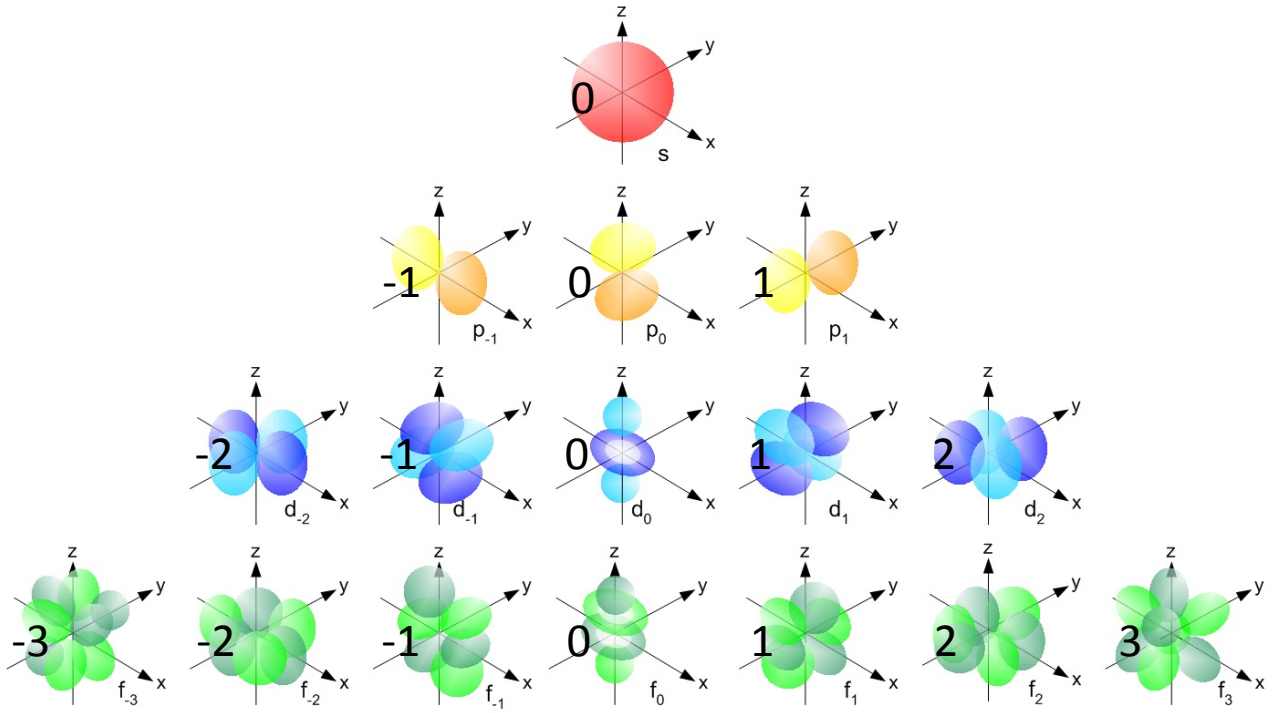
$n = 1, 2, 3\ldots$ $\quad l = 0, 1 \ldots n\text{-}1$ $\quad m_l = -l \ldots 0 \ldots l$ $\quad m_s = ½, -½$

n	l	m_l
1	0	0
2	1	-1, 0 , 1
	0	0
3	2	-2, -1, 0 , 1, 2
	1	-1, 0 , 1
	0	0
4	3	-3, -2, -1, 0 , 1, 2, 3
	2	-2, -1, 0 , 1, 2
	1	-1, 0 , 1
	0	0

Quantum Numbers:

Orbital Nomenclature:

n	l	m_l	
1	0	0	1s
2	1	-1, 0, 1	2p
3	2	-2, -1, 0, 1, 2	3d
4	3	-3, -2, -1, 0, 1, 2, 3	4f



http://chemwiki.ucdavis.edu/Physical_Chemistry/Quantum_Mechanics/Atomic_Theory/Electrons_in_Atoms/Electronic_Orbitals

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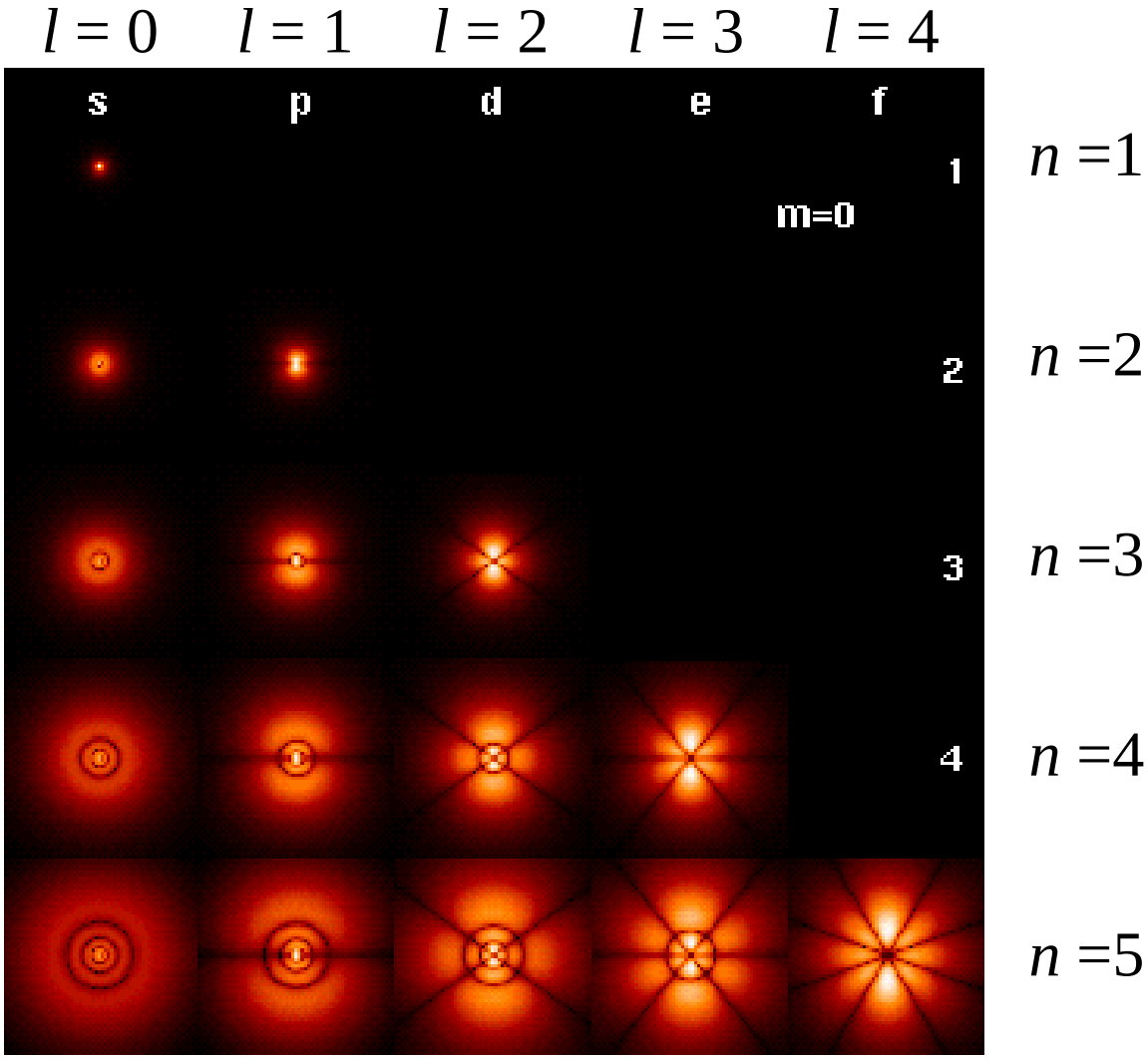

http://en.wikipedia.org/wiki/Hydrogen_atom

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- Quantum mechanics is necessary to describe:
  - Electron densities
  - Bonding
  - electronic, optical, magnetic properties

- "Quantum numbers" come from solution to Schroedinger equation
  - Describe electron density/energy levels
  - "orbitals"

- n – principal quantum number (shell)
- l – angular momentum/azimuthal quantum number (orbital)
- m_l – magnetic quantum number (orientation)
- m_s – spin quantum number (spin up/down)