

Homework IP/EA of Atoms

Periodic Table of Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1 H Hydrogen 1.00794	Atomic # Symbol Name Atomic Mass																2 He Helium 4.002602	
2	3 Li Lithium 6.941	4 Be Beryllium 9.012182	C Solid Hg Liquid H Gas Rf Unknown Metals Alkali metals Alkaline earth metals Lanthanoids Actinoids Transition metals Poor metals Other nonmetals Noble gases										5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.0067	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797	
3	11 Na Sodium 22.98976928	12 Mg Magnesium 24.3050											13 Al Aluminium 26.9815386	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948	
4	19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798	
5	37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.96	43 Tc Technetium (97.9072)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.293	
6	55 Cs Caesium 132.9054519	56 Ba Barium 137.327	57–71																86 Rn Radon (222.0178)
7	87 Fr Francium (223)	88 Ra Radium (226)	89–103																118 Uuo Ununoctium (294)
				72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98040	84 Po Polonium (209.9824)	85 At Astatine (209.9871)	86 Rn Radon (222.0178)	
				104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Uub Ununbium (285)	113 Uut Ununtrium (284)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (292)	117 Uus Ununseptium	118 Uuo Ununoctium (294)	

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

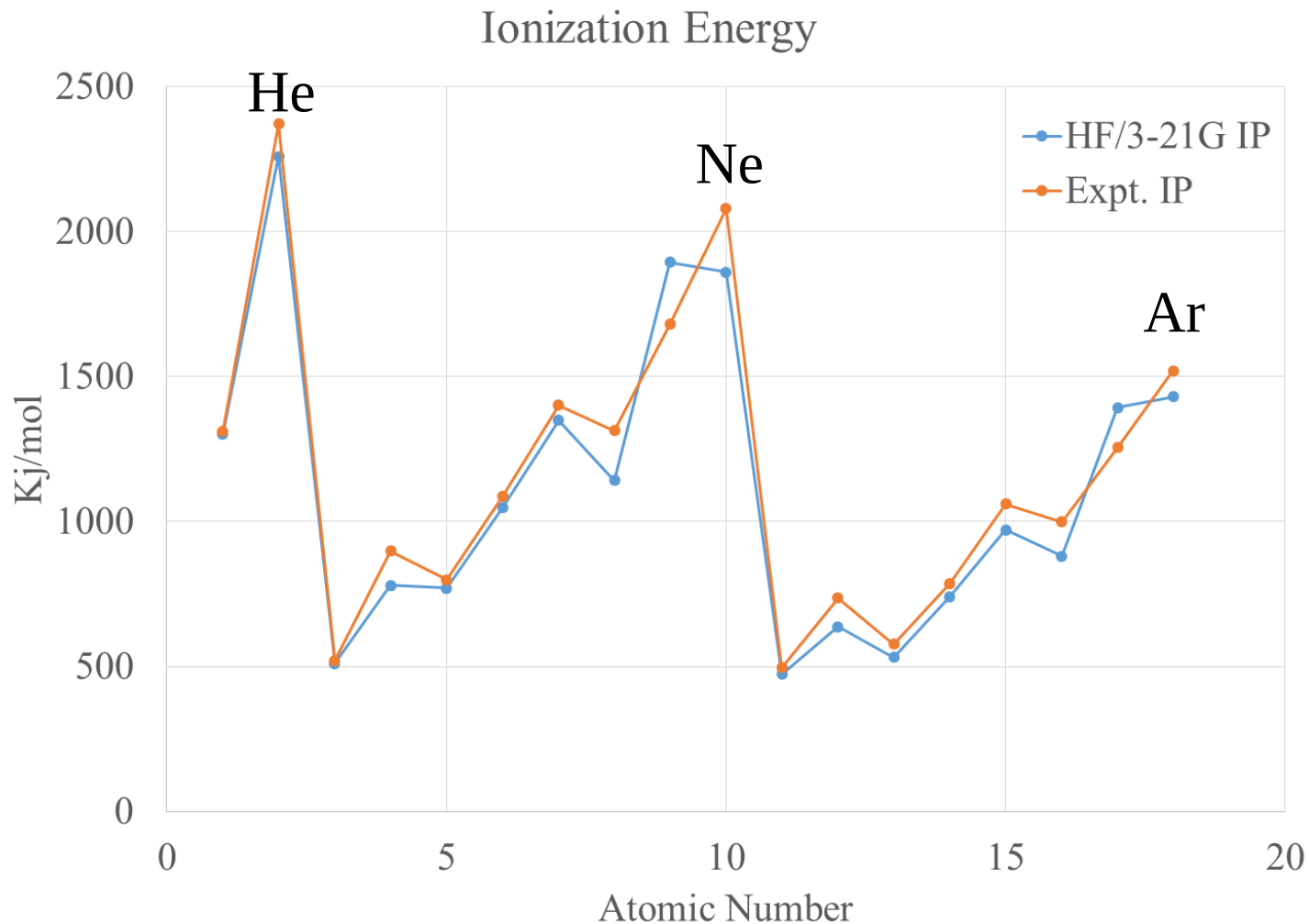
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57 La Lanthanum 138.90547	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93032	68 Er Erbium 167.259	69 Tm Thulium 168.93421	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.9668
89 Ac Actinium (227)	90 Th Thorium 232.03806	91 Pa Protactinium 231.03588	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

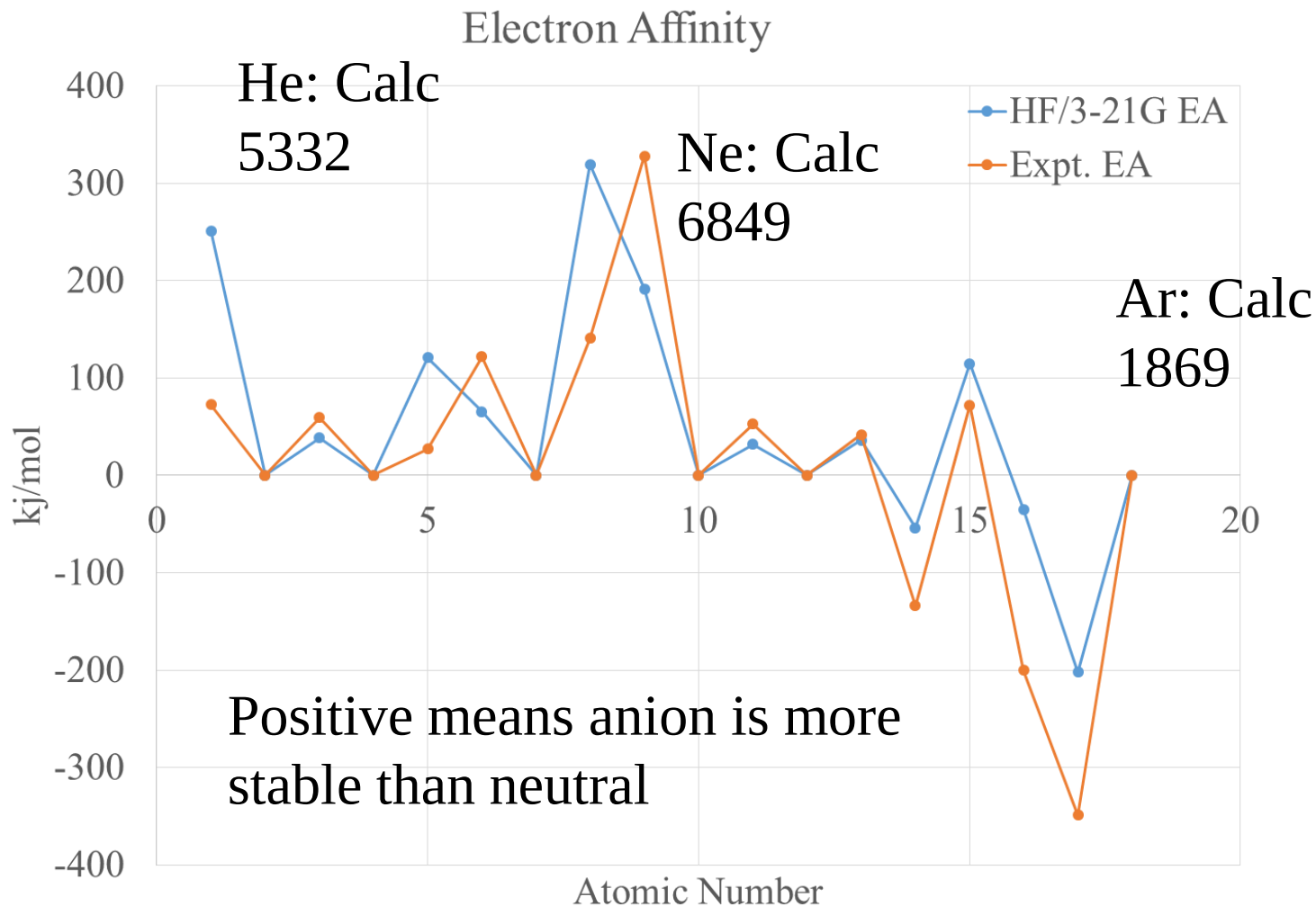
Results?

	IP	kJ/mol	EA	kJ/mol	2nd IP	kJ/mol	3rd IP	kJ/mol
	HF/3- 21G	Exp	HF/3- 21G	Exp	HF/3- 21G	Exp	HF/3- 21G	Exp
Ne	1860	2081	6849		4356	3952		
Na	473	496	-32	-53	4583	4562		
Fe	686	759	223	15	2002	1561		
Mo			127	72			4196	3891
I	909	1008	191	295				
Cs	335	376	-44	46	2204	2234		

Calculated Ionization Energies



Calculated Electron Affinities



In this plot the ones without experiment are made zero

H_2^+ molecule

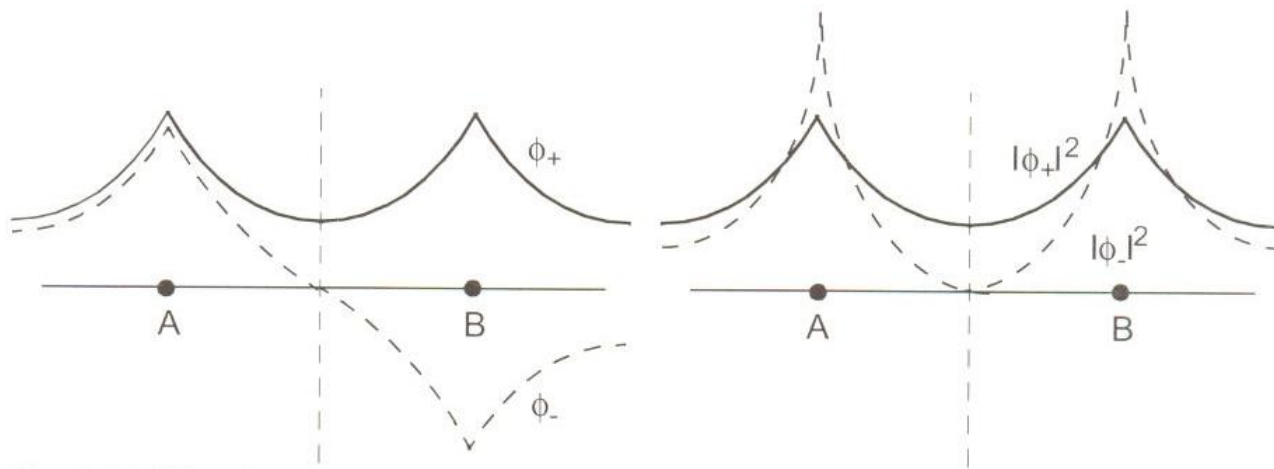
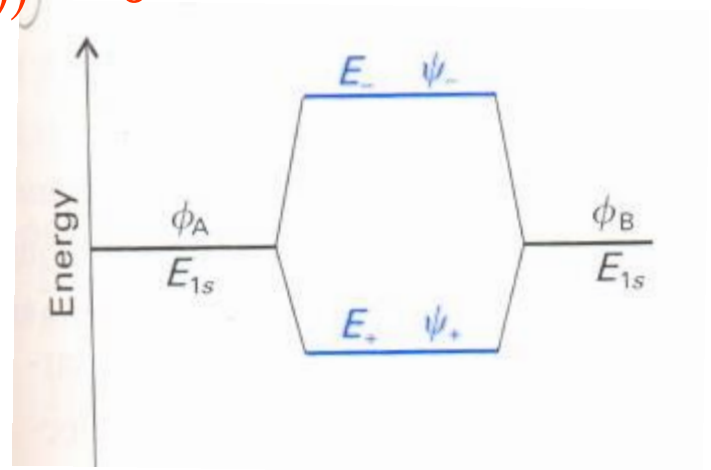
Solve Secular Equation

$$\begin{vmatrix} H(R)_{AA} - E(R) & H(R)_{AB} - E(R)S \\ H(R)_{BA} - E(R)S & H(R)_{BB} - E(R) \end{vmatrix} = 0$$

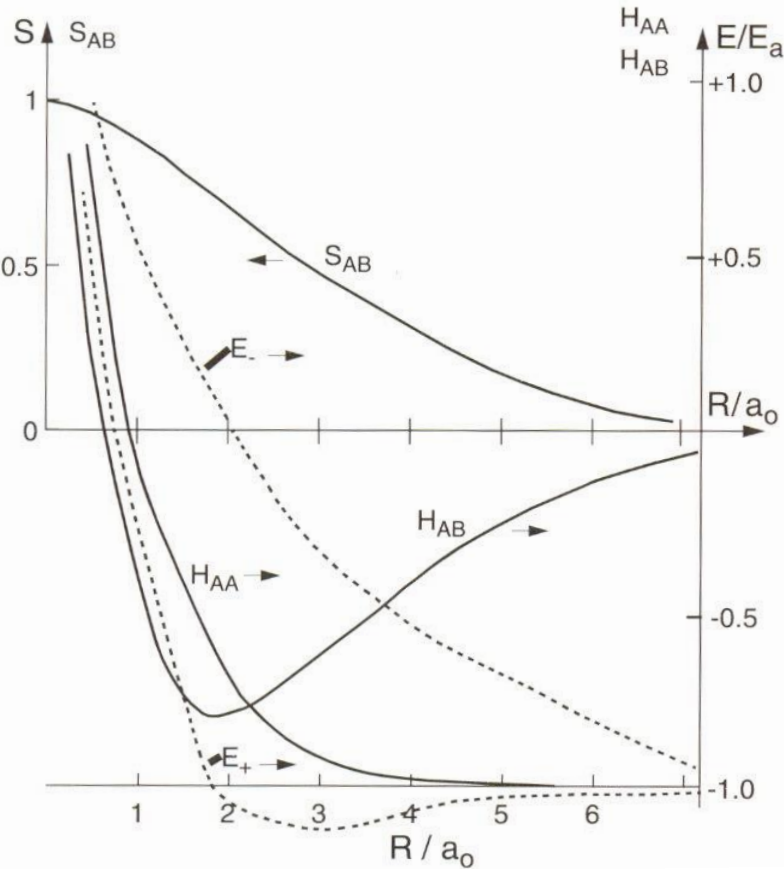
$$(H(R)_{AA} - E(R))^2 - (H(R)_{BA} - E(R)S(R))^2 = 0$$

$$E_{\pm}(R) = \frac{H(R)_{AA} \pm H(R)_{AB}}{1 \pm S(R)}$$

$$\Psi_{\pm} = |\pm\rangle = \frac{|A\rangle \pm |B\rangle}{\sqrt{2 \pm 2S}}$$



Energy Lowering and Rising



At equilibrium of E_+

$$H_{AA}, H_{AB} < 0; S > 0$$

$$\text{Lowering} = H_{AA} - E_+ \quad \text{Rising} = E_- - H_{AA}$$

$$= H_{AA} - \frac{H_{AA} + H_{AB}}{1 + S} = \frac{H_{AA} - H_{AB}}{1 - S} - H_{AA}$$

$$= \frac{SH_{AA} - H_{AB}}{1 + S} = \frac{SH_{AA} - H_{AB}}{1 - S}$$

Is energy of lowering much more than the energy of rising? ΔE

$$\Delta E = \frac{SH_{AA} - H_{AB}}{1 - S} - \frac{SH_{AA} - H_{AB}}{1 + S} =$$

If $S=0$ then $\Delta E=0$, $S>0$ then $\Delta E>0$ rising is more than lowering!

Bonding Orbital Compare With Exact

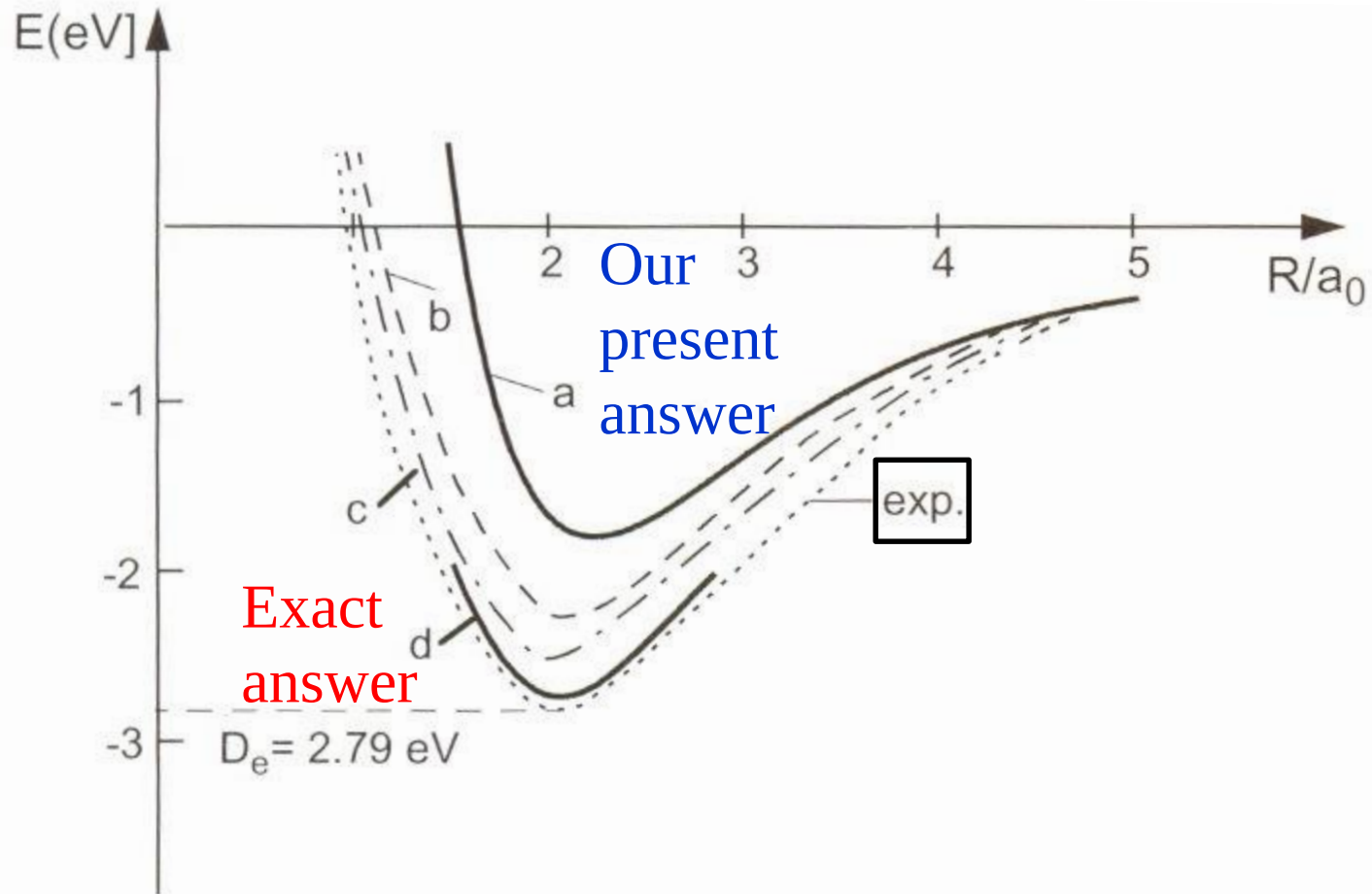


Fig. 2.30 Potential curve of the H_2^+ ground state as computed with a) simple LCAO, b) optimized parameter η , c) polarization term, and d) exact treatment.

Antibonding Orbital

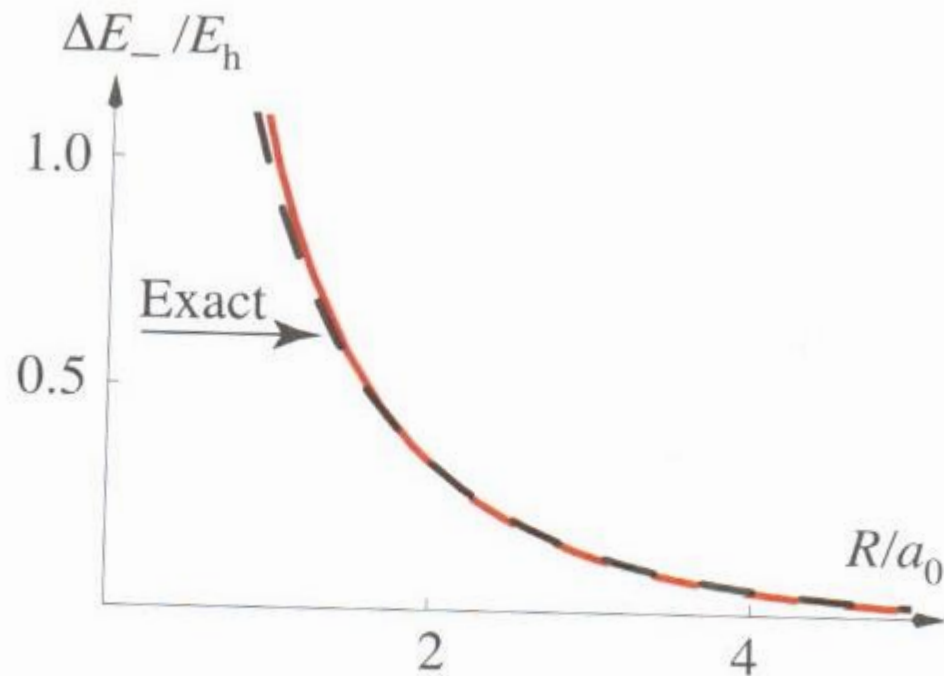


FIGURE 10.13

comparison of the energy $\Delta E_-(R)$ of the first excited state of H_2^+ calculated from equation 10.23 with the exact energy.

Additional Orbitals

TABLE 10.2

Results of Various Calculations of the Ground-State Electronic Energy of H_2^+ ^a

ϕ	$E_{\min}/E_{\text{h}}$	R_{eq}/a_0
$1s(\zeta = 1.000)$	-0.564 83	2.49
$1s(\zeta = 1.238)$	-0.586 51	2.00
$1s(\zeta = 1.000) + a2p_z(\zeta = 1.000)$	-0.565 91	2.00
$1s(\zeta = 1.247) + b2p_z(\zeta = 1.247)$	-0.599 07	2.00
$1s(\zeta = 1.2458) + c2p_z(\zeta = 1.4224)$	-0.600 36	2.00
$1s(\zeta = 1.244) + c_1 2p_z(\zeta = 1.152) + c_2 3d_{z^2}(\zeta = 1.333)$ ^b	-0.6020	2.00
Exact ^c	-0.602 64	2.00

^a The molecular orbitals are of the form $\psi_{\text{b}} = c_{\text{A}}\phi_{\text{A}} + c_{\text{B}}\phi_{\text{B}}$, where ϕ is given in the table.

^b Mulliken, R. S., Ermler, W. C. *Diatomic Molecules*. Academic Press: New York, 1977.

^c Bates, D. R., Ledsham, K., Stewart, A. L. Wave Functions of the Hydrogen Molecular Ion. *Philos. Trans. Roy. Soc. London, Ser. A*. **246**, 215 (1953).

Bonding Orbital Compare With Exact

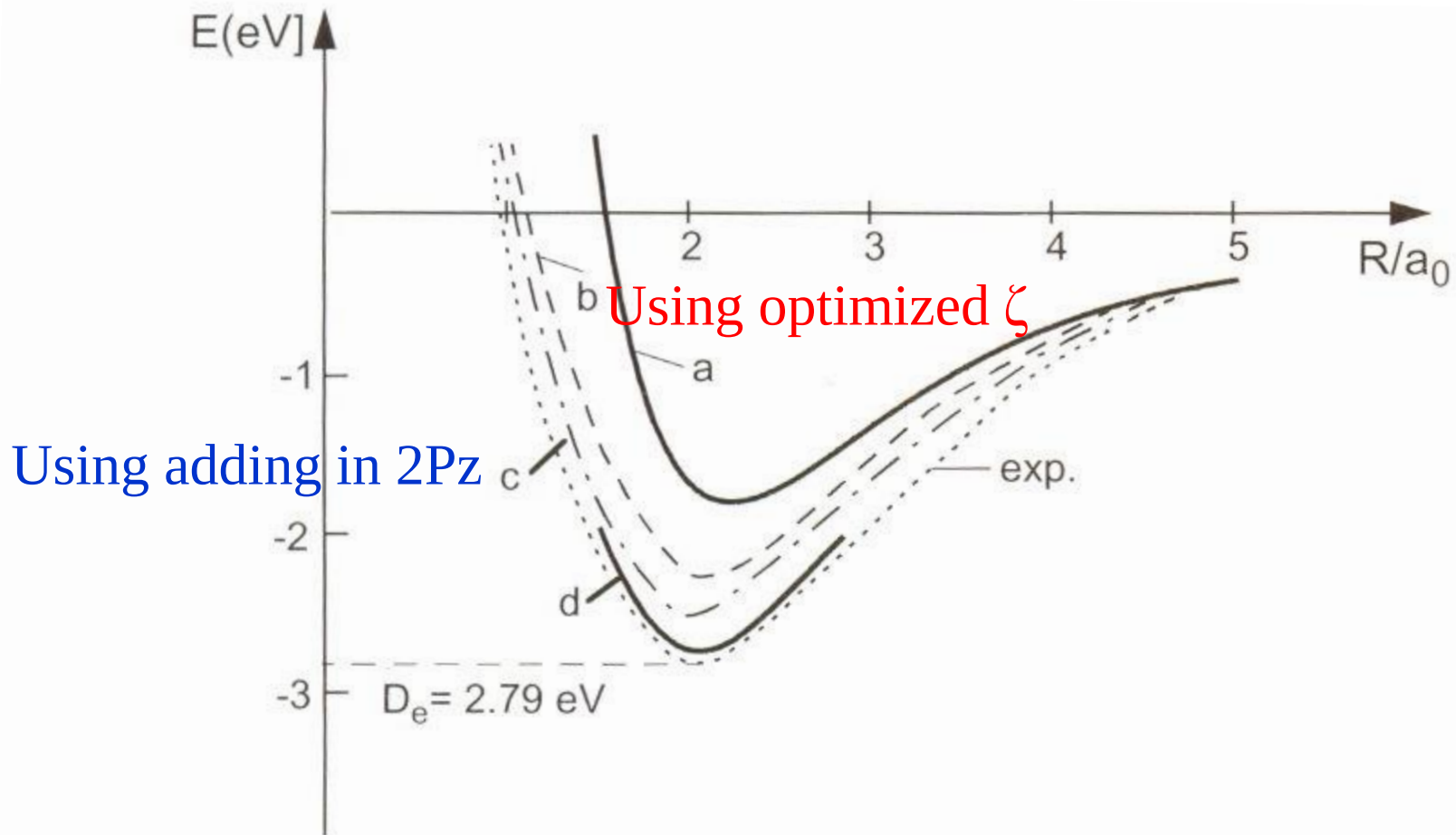


Fig. 2.30 Potential curve of the H_2^+ ground state as computed with a) simple LCAO, b) optimized parameter η , c) polarization term, and d) exact treatment.

Basis Set

- If you use more atomic orbitals to define the molecular orbital usually the energy gets closer to the exact solution



Using a bigger basis set to describe the system

- However bigger basis set you need more time to calculate.
- Changing coefficient on basis set is also important

Addition of Orbitals

$$\Psi_n^{el}(\mathbf{r}) = \sum_i^n C_i \psi_i(\mathbf{r})$$

Adding in the contribution from 2S

$$\begin{aligned}\Psi_n^{el}(\mathbf{r}; R) &= C_1 |A1s\rangle + C_2 |B1s\rangle + C_3 |A2s\rangle + C_4 |B2s\rangle \\ &= 0.7071(|A1s\rangle + |B1s\rangle) + 0.00145(|A2s\rangle + |B2s\rangle)\end{aligned}$$

Adding in the contribution from 2p_z

$$\begin{aligned}\Psi_n^{el}(\mathbf{r}; R) &= C_1 |A1s\rangle + C_2 |B1s\rangle + C_3 |A2p_z\rangle + C_4 |B2p_z\rangle \\ &= C_A(|A1s\rangle + 0.1380|A1p_z\rangle) + C_B(|B1s\rangle + 0.1380|B1p_z\rangle)\end{aligned}$$

Questions

- Why does using a smaller atomic wavefunction help?
- Why does adding a 2p orbital help in making the energy lower, but adding the 2s orbital does not help much?

Diatomic Molecules

H₂

$$\begin{aligned}
 & \hat{H}\Psi_n^{el}(\mathbf{r}_1, \mathbf{r}_2; R) \\
 &= \left[-\frac{1}{2}\nabla_1^2 + -\frac{1}{2}\nabla_2^2 + \left[\frac{1}{|\mathbf{R}|} - \frac{1}{|\mathbf{r}_{1A}|} - \frac{1}{|\mathbf{r}_{1B}|} - \frac{1}{|\mathbf{r}_{2A}|} - \frac{1}{|\mathbf{r}_{2B}|} + \frac{1}{|\mathbf{r}_{12}|} \right] \right] \Psi_n^{el}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{R}) \\
 &= E_n(\mathbf{R})\Psi_n^{el}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{R})
 \end{aligned}$$

Above equation ?

$$\begin{aligned}
 &= \left[-\frac{1}{2}\nabla_1^2 - \frac{1}{|\mathbf{r}_{1A}|} - \frac{1}{|\mathbf{r}_{1B}|} - \frac{1}{2}\nabla_2^2 - \frac{1}{|\mathbf{r}_{2A}|} - \frac{1}{|\mathbf{r}_{2B}|} + \left[\frac{1}{|\mathbf{R}|} + \frac{1}{|\mathbf{r}_{12}|} \right] \right] \Psi_n^{el}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{R}) \\
 &= \left[h_1 + h_2 + \frac{1}{|\mathbf{R}|} + \frac{1}{|\mathbf{r}_{12}|} \right] \Psi_n^{el}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{R})
 \end{aligned}$$

Spin Orbital and Spacial Orbitals

When you consider more than one electron you have to consider not only the $\mathbf{r}$ but also the spin s and the Fermi principle:

Define $\mathbf{x}$ as the summed coordinate for $\mathbf{r}$ and s

$$\psi_i(\mathbf{x}) = \psi_i(\mathbf{r}, s) = \phi_a(\mathbf{r}) \begin{matrix} \alpha(s) \\ \beta(s) \end{matrix}$$

Hartree Product $\Psi^{HP}(\mathbf{x}_1, \mathbf{x}_2) = \psi_i(\mathbf{x}_1) \psi_j(\mathbf{x}_2)$

However the above does not satisfy the ?

Exchange of electron leads to asymmetric wave function

?

Slater Determinant

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} (\psi_i(\mathbf{x}_1)\psi_j(\mathbf{x}_2) - \psi_j(\mathbf{x}_1)\psi_i(\mathbf{x}_2))$$

$$\Psi(\mathbf{x}_2, \mathbf{x}_1) = ?$$

Asymmetric wavefunction after exchange of electron coordinate

Generalization for n electron system: Slater Determinant

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_i(\mathbf{x}_1) & \psi_j(\mathbf{x}_1) & \dots & \psi_k(\mathbf{x}_1) \\ \psi_i(\mathbf{x}_2) & \psi_j(\mathbf{x}_2) & \dots & \psi_k(\mathbf{x}_2) \\ \dots & \dots & \dots & \dots \\ \psi_i(\mathbf{x}_n) & \psi_j(\mathbf{x}_n) & \dots & \psi_k(\mathbf{x}_n) \end{vmatrix}$$

As an educator and advisor

[\[edit\]](#)

Slater's concern for the well being of others is well illustrated by the following dialog that [Richard Feynman](#) relates. It took place at the end of his undergraduate days at MIT, when he wanted to stay on to do a Ph.D.^[81] "When I went to Professor Slater and told him of my intentions he said: 'We will not have you here'. I said 'What?' Slater said 'Why do you think you should go to graduate school at MIT?' 'Because it is the best school for science in the country' ... 'That is why you should go to some other school. You should find out how the rest of the world is.' So I went to Princeton. ... Slater was right. And I often advise my students the same way. Learn what the rest of the world is like. The variety is worth while."

Summary

[\[edit\]](#)

From the memoir by Philip Morse: "He contributed significantly to the start of the quantum revolution in physics; he was one of the very few American-trained physicists to do so. He was exceptional in that he persisted in exploring atomic, molecular and solid state physics, while many of his peers were coerced by war, or tempted by novelty, to divert to nuclear mysteries. Not least, his texts and his lectures contributed materially to

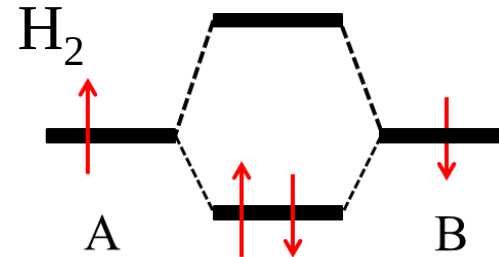
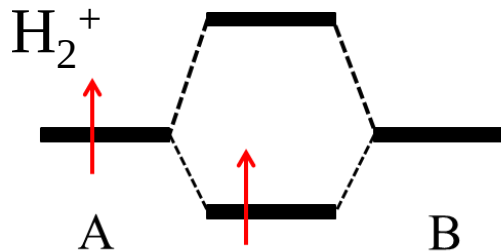
What Happens if we use direct product of H_2^+ solutions

$$|+\rangle = \frac{|A\rangle + |B\rangle}{\sqrt{2 + 2S}}$$

$$|\Psi_{trial}\rangle = \frac{1}{\sqrt{2!}} \begin{vmatrix} \alpha(1)|+\rangle_1 & \beta(1)|+\rangle_1 \\ \alpha(2)|+\rangle_2 & \beta(2)|+\rangle_2 \end{vmatrix}$$

$$= |+\rangle_1 |+\rangle_2 \left[\frac{1}{\sqrt{2}} (\alpha(1)\beta(2) - \alpha(2)\beta(1)) \right]$$

?



Hamiltonian does not include any spin terms so we could obtain the R dependence of the energy using only the spatial part of the electronic wavefunction

$${}_2\langle + |_1 \langle + | \hat{H} | + \rangle_1 | + \rangle_2 (R)$$

Potential Energy Curve

$${}_2\langle + | {}_1\langle + | \hat{H} | + \rangle {}_1 | + \rangle {}_2 (R)$$

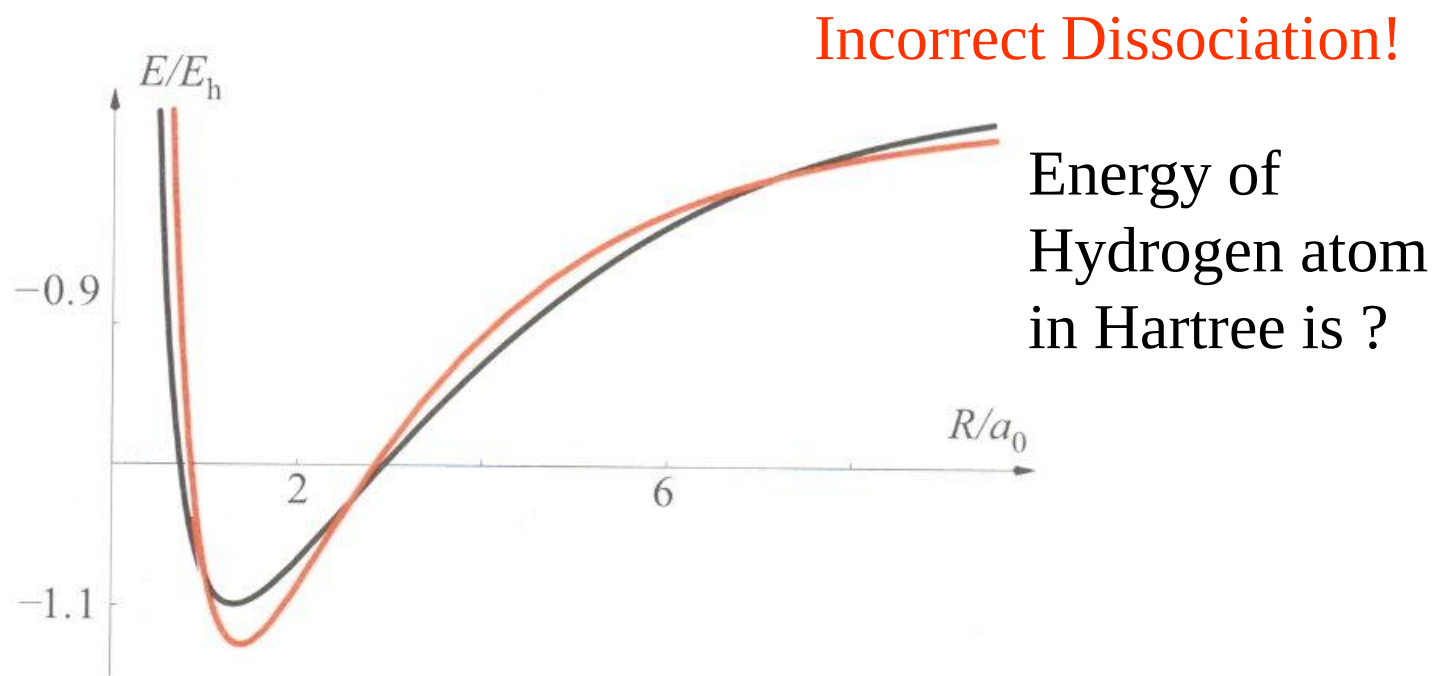


FIGURE 10.23

Both the optimized (orange) and the $\zeta = 1$ (black) molecular orbital energies calculated with Equation 10.41. In neither case does the energy go to the correct limit of $-1 E_h$ as $R \rightarrow \infty$.

What is the Problem of incorrect dissociation

$$\begin{aligned}
 |+\rangle_1 |+\rangle_2 &\approx (|A1s\rangle_1 + |B1s\rangle_1) \times (|A1s\rangle_2 + |B1s\rangle_2) \\
 &= |A1s\rangle_1 |A1s\rangle_2 + |B1s\rangle_1 |B1s\rangle_2 + |A1s\rangle_1 |B1s\rangle_2 + |B1s\rangle_1 |A1s\rangle_2
 \end{aligned}$$

First two terms have 2 electrons on one of the atoms: IONIC

Last two terms have one electrons on each one of the atoms:
Valance Bond

$$|+\rangle_1 |+\rangle_2 \approx |I\rangle + |VB\rangle$$

Solution: Configuration Interaction

Two 1S orbitals can make **TWO** molecular orbitals:
bonding and antibonding!

Why not use the two and make combinations 2e⁻ in antibond

$$|\Psi_1\rangle = C_1 \begin{vmatrix} \alpha(1)|+\rangle_1 & \beta(1)|+\rangle_1 \\ \alpha(2)|+\rangle_2 & \beta(2)|+\rangle_2 \end{vmatrix}$$

$$|\Psi_2\rangle = C_2 \begin{vmatrix} \alpha(1)|-\rangle_1 & \beta(1)|-\rangle_1 \\ \alpha(2)|-\rangle_2 & \beta(2)|-\rangle_2 \end{vmatrix}$$

$$|\Psi_1\rangle \approx |++\rangle(\alpha\beta - \beta\alpha) \quad \text{2e⁻ in bond}$$

$$|\Psi_2\rangle \approx |--\rangle(\alpha\beta - \beta\alpha)$$

1e⁻ in bond; 1e⁻ in antibond

$$|\Psi_3\rangle = C_3 \begin{vmatrix} \alpha(1)|+\rangle_1 & \alpha(1)|-\rangle_1 \\ \alpha(2)|+\rangle_2 & \alpha(2)|-\rangle_2 \end{vmatrix}$$

$$|\Psi_4\rangle = C_4 \begin{vmatrix} \alpha(1)|+\rangle_1 & \beta(1)|-\rangle_1 \\ \alpha(2)|+\rangle_2 & \beta(2)|-\rangle_2 \end{vmatrix}$$

$$|\Psi_3\rangle \approx (|+-\rangle - |-+\rangle)\alpha\alpha$$

$$|\Psi_4\rangle \approx |+-\rangle\alpha\beta - |-+\rangle\beta\alpha$$

$$|\Psi_5\rangle = C_5 \begin{vmatrix} \beta(1)|+\rangle_1 & \alpha(1)|-\rangle_1 \\ \beta(2)|+\rangle_2 & \alpha(2)|-\rangle_2 \end{vmatrix}$$

$$|\Psi_6\rangle = C_6 \begin{vmatrix} \beta(1)|+\rangle_1 & \beta(1)|-\rangle_1 \\ \beta(2)|+\rangle_2 & \beta(2)|-\rangle_2 \end{vmatrix}$$

$$|\Psi_5\rangle \approx |+-\rangle\beta\alpha - |-+\rangle\alpha\beta$$

$$|\Psi_6\rangle \approx (|+-\rangle - |-+\rangle)\beta\beta$$

Symmetry of Spacial Orbitals

$$|\Psi_1\rangle \approx |++\rangle(\alpha\beta - \beta\alpha)$$

$$|\Psi_2\rangle \approx |--\rangle(\alpha\beta - \beta\alpha)$$

$$|\Psi_3\rangle \approx (|+-\rangle - |-+\rangle)\alpha\alpha$$

$$|\Psi_4\rangle \approx |+-\rangle\alpha\beta - |-+\rangle\beta\alpha$$

$$|\Psi_5\rangle \approx |+-\rangle\beta\alpha - |-+\rangle\alpha\beta$$

$$|\Psi_6\rangle \approx (|+-\rangle - |-+\rangle)\beta\beta$$

If you exchange the position of electron 1 and electron 2

$$|\Psi_1\rangle \text{ and } |\Psi_2\rangle ?$$

$$|\Psi_3\rangle \text{ and } |\Psi_4\rangle \text{ and } |\Psi_5\rangle \text{ and } |\Psi_6\rangle ?$$

Hamiltonian is ?

$$H = \left[-\frac{1}{2} \nabla_1^2 + -\frac{1}{2} \nabla_2^2 + \left[\frac{1}{|\mathbf{R}|} - \frac{1}{|\mathbf{r}_{1A}|} - \frac{1}{|\mathbf{r}_{1B}|} - \frac{1}{|\mathbf{r}_{2A}|} - \frac{1}{|\mathbf{r}_{2B}|} + \frac{1}{|\mathbf{r}_{12}|} \right] \right]$$

Solution: Configuration Interaction

Using an wavefunction with two electrons in bonding orbital as well as two electrons in antibonding orbital

$$|\Psi_1\rangle = C_1 \begin{vmatrix} \alpha(1)|+\rangle_1 & \beta(1)|+\rangle_1 \\ \alpha(2)|+\rangle_2 & \beta(2)|+\rangle_2 \end{vmatrix}$$

$$|\Psi_1\rangle \approx |++\rangle(\alpha\beta - \beta\alpha)$$

Configuration 1: ?

$$|\Psi_2\rangle = C_2 \begin{vmatrix} \alpha(1)|-\rangle_1 & \beta(1)|-\rangle_1 \\ \alpha(2)|-\rangle_2 & \beta(2)|-\rangle_2 \end{vmatrix}$$

$$|\Psi_2\rangle \approx |--\rangle(\alpha\beta - \beta\alpha)$$

Configuration 2: ?

Configuration Interaction

$$|\Psi_{CI}\rangle = C_1|\Psi_1\rangle + C_2|\Psi_2\rangle = C_1|++\rangle + C_2|--\rangle$$

$$\begin{aligned} |++\rangle &\approx (|A1s\rangle_1 + |B1s\rangle_1) \times (|A1s\rangle_2 + |B1s\rangle_2) \\ &= |A1s\rangle_1 |A1s\rangle_2 + |B1s\rangle_1 |B1s\rangle_2 + |A1s\rangle_1 |B1s\rangle_2 + |B1s\rangle_1 |A1s\rangle_2 \\ |--\rangle &\approx (|A1s\rangle_1 - |B1s\rangle_1) \times (|A1s\rangle_2 - |B1s\rangle_2) \\ &= |A1s\rangle_1 |A1s\rangle_2 + |B1s\rangle_1 |B1s\rangle_2 - |A1s\rangle_1 |B1s\rangle_2 - |B1s\rangle_1 |A1s\rangle_2 \end{aligned}$$

$$|\Psi_{CI}\rangle = C_1|\Psi_1\rangle + C_2|\Psi_2\rangle = ?$$

?

H2 Potential Curve Revisited

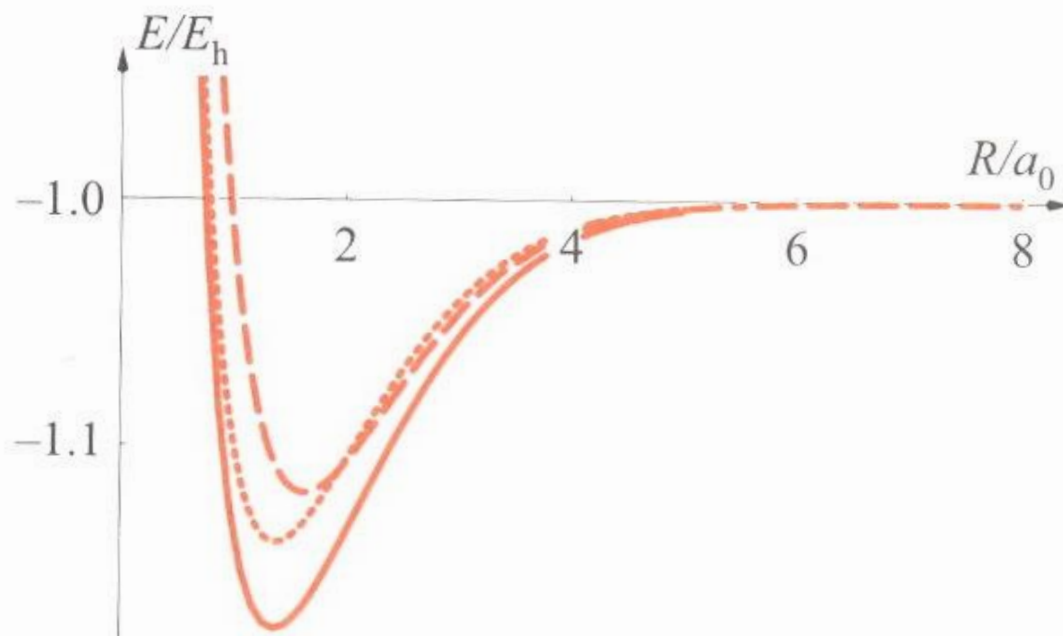


FIGURE 10.25

The configuration-interaction energy E_{CI} of the ground-state energy of H_2 for $\zeta = 1$ (dashed curve) and for an optimized value of ζ (dotted curve) plotted against R . The “exact” results of Kolos and Wolniewicz (solid curve) are shown for comparison.

R Dependence of Expansion Coefficients

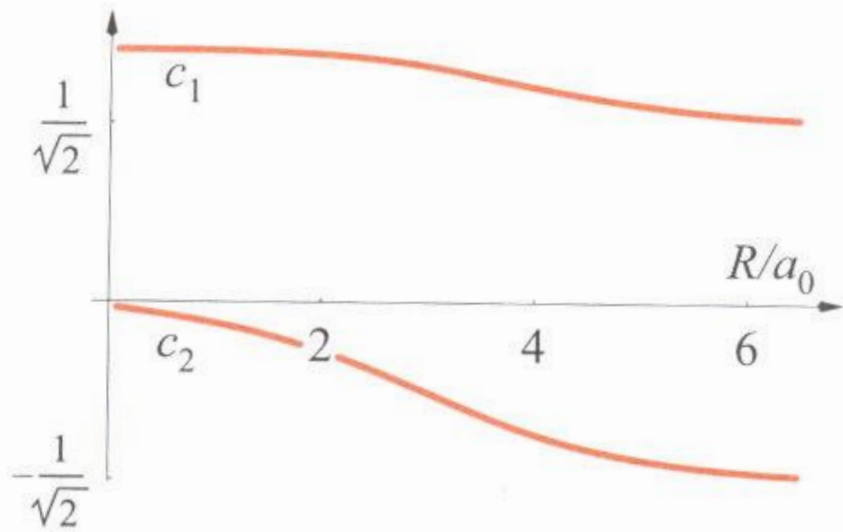


FIGURE 10.27

A plot of c_1 and c_2 for the optimized value of ζ in Equation 10.53 against R . Note that $c_1 \rightarrow 1/\sqrt{2}$ and $c_2 \rightarrow -1/\sqrt{2}$ as $R \rightarrow \infty$.

Use of more orbitals

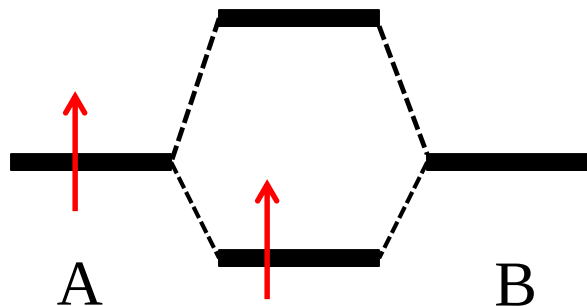
$$|\pm\rangle \approx C_A(|A1s\rangle + \alpha|A1p_z\rangle) \pm C_B(|B1s\rangle + \alpha|B1p_z\rangle)$$

TABLE 10.4

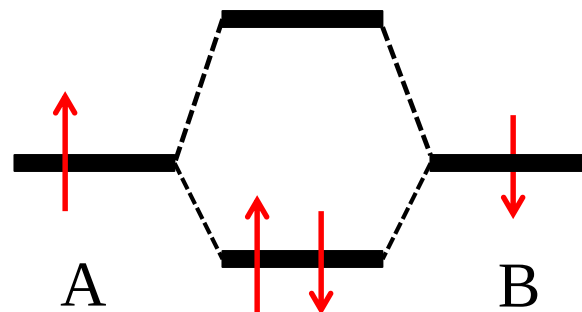
Results of Various Calculations of the Ground-State Energy of H₂

	Wave function	ζ	$E_{\min}/E_h$	R_{eq}/a_0
MO	Minimal basis set	1.000	-1.0991	1.603
MO	Minimal basis set	1.193	-1.1282	1.385
	Hartree-Fock ^a		-1.1336	1.400
CI	Minimal basis set	1.000	-1.1187	1.668
CI	Minimal basis set	1.194	-1.1479	1.430
CI	Minimal basis set with polarization ^b		-1.1514	1.40
CI	Five terms ^b		-1.1672	1.40
CI	33 terms ^c		-1.1735	1.40
	Trial function with r_{12} 13 terms ^d		-1.1735	1.40
	Trial function with r_{12} with 100 terms ^e		-1.1744	1.401
	Experimental ^f		-1.174	1.401

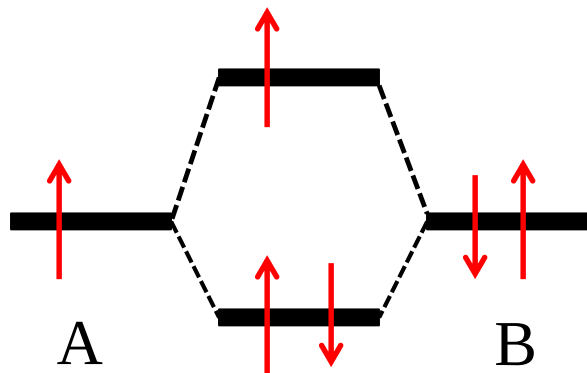
H_2^+ , H_2 , He_2^+ , He_2



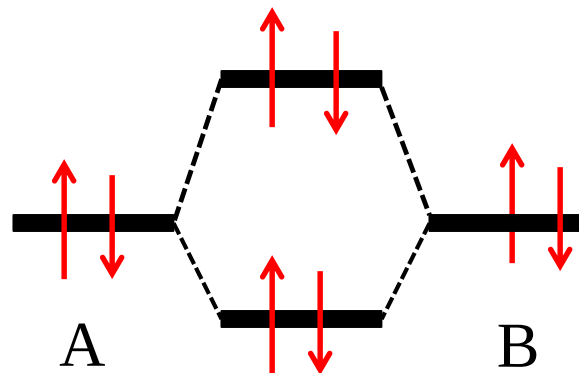
H_2^+ $R_{\text{eq}} = 1.06$ Angstrom
 Binding Energy 61 kcal/mol



H_2 $R_{\text{eq}} = ?$ Angstrom
 Binding Energy ? kcal/mol



He_2^+ $R_{\text{eq}} = ?$ Angstrom
 Binding Energy ? kcal/mol



He_2 $R_{\text{eq}} = \text{Infinity}$ not bound
 Binding Energy 0 Kcal mol