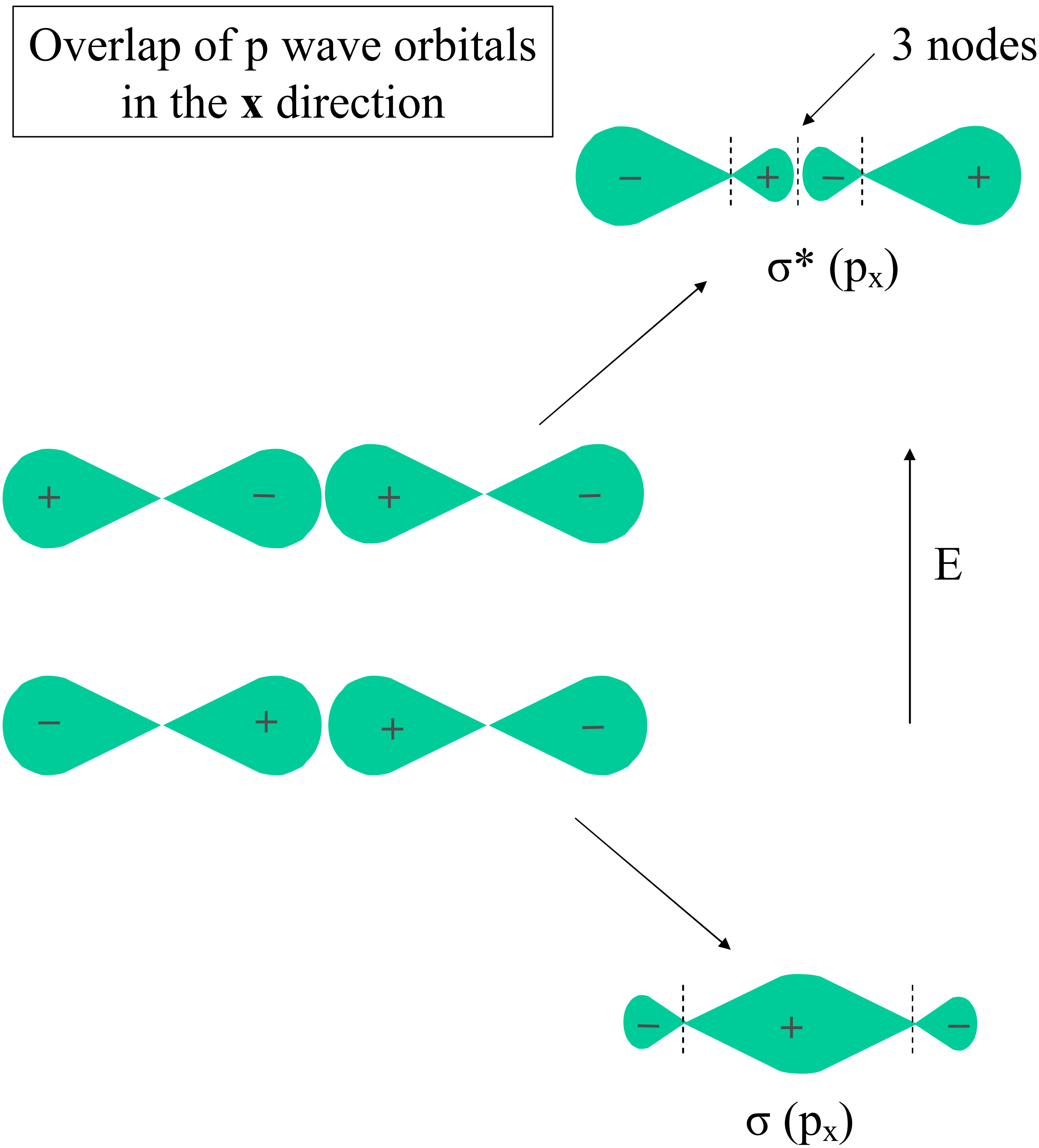

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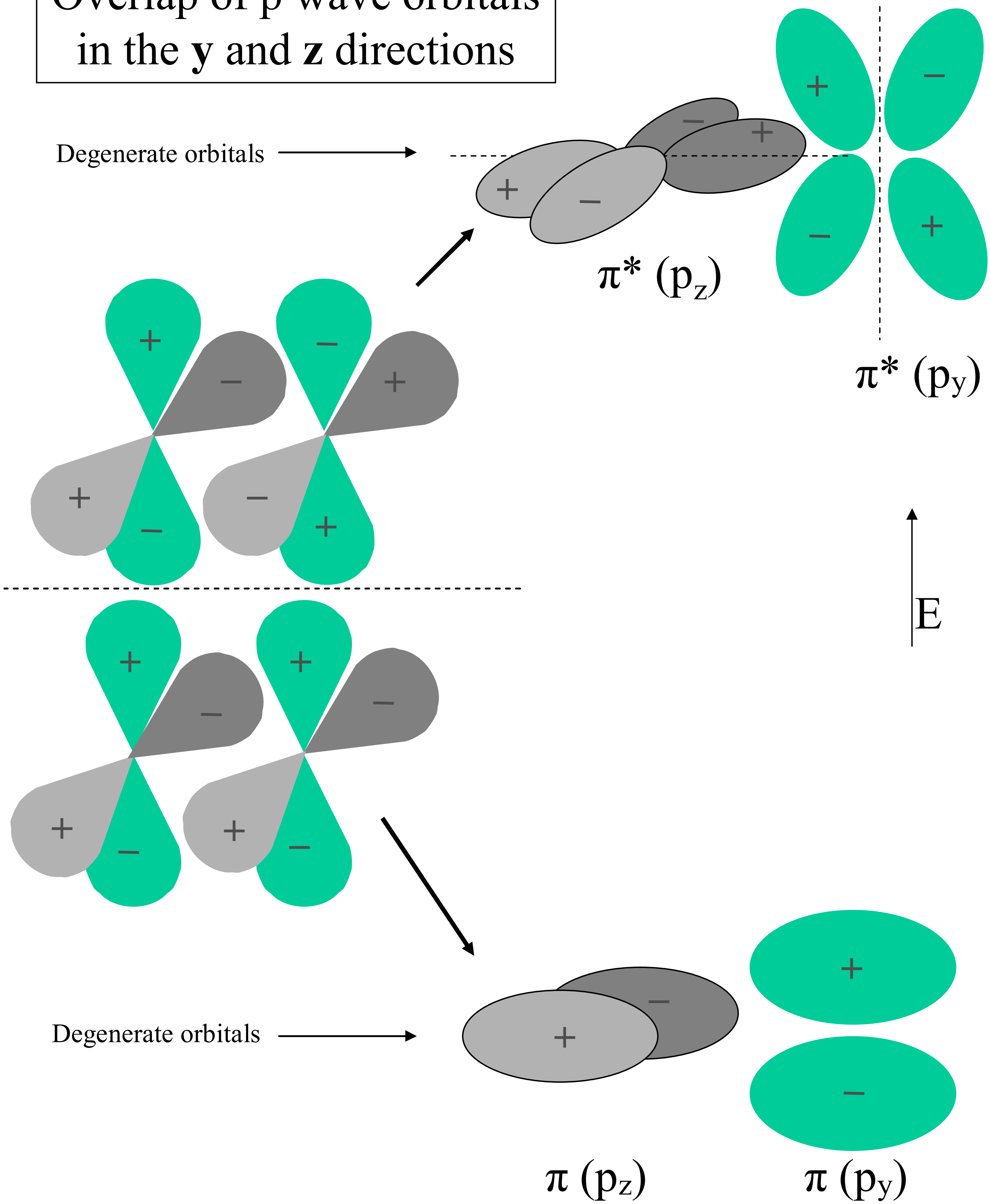
Overlap of p wave orbitals in the **y** and **z** directions



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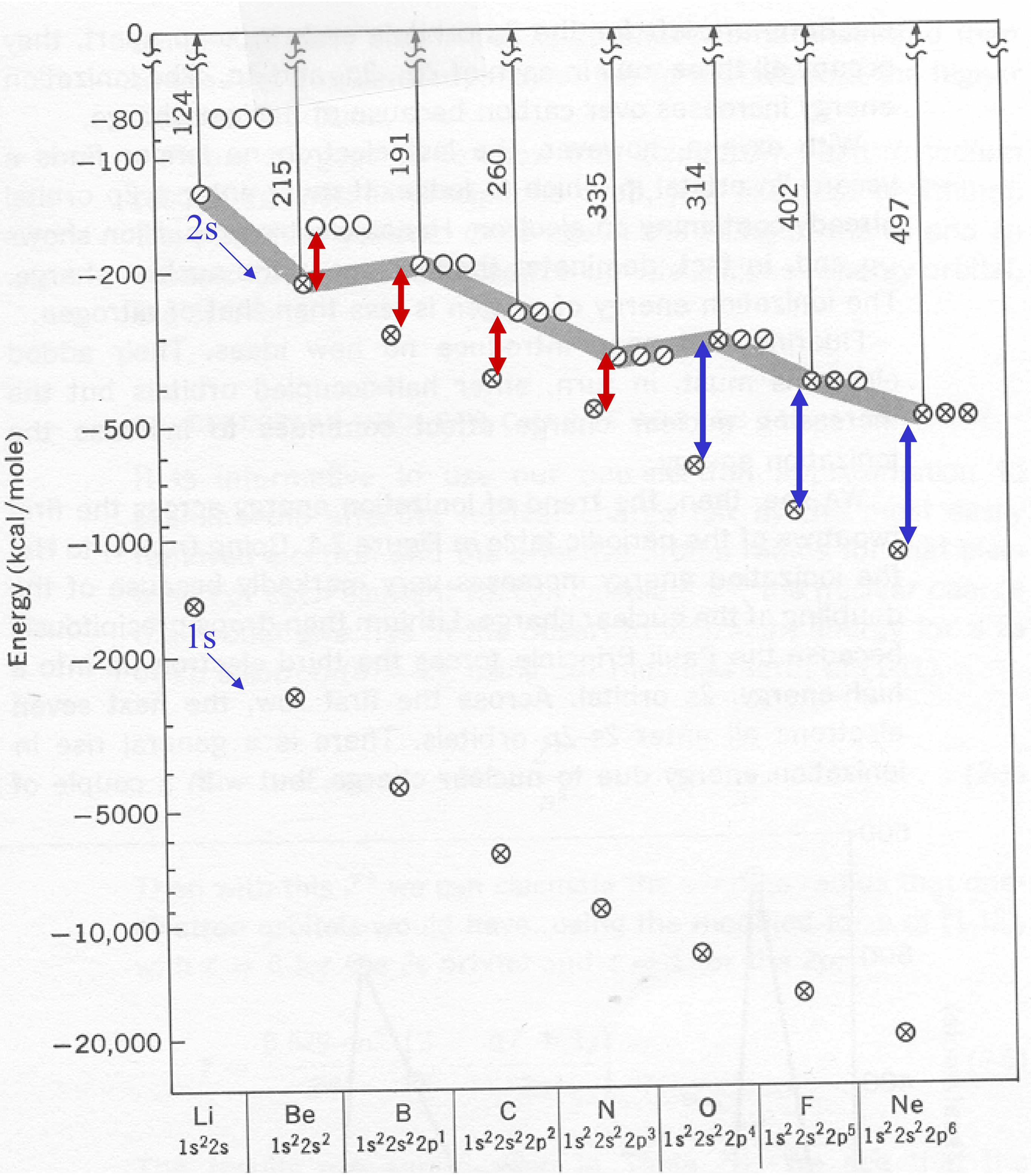
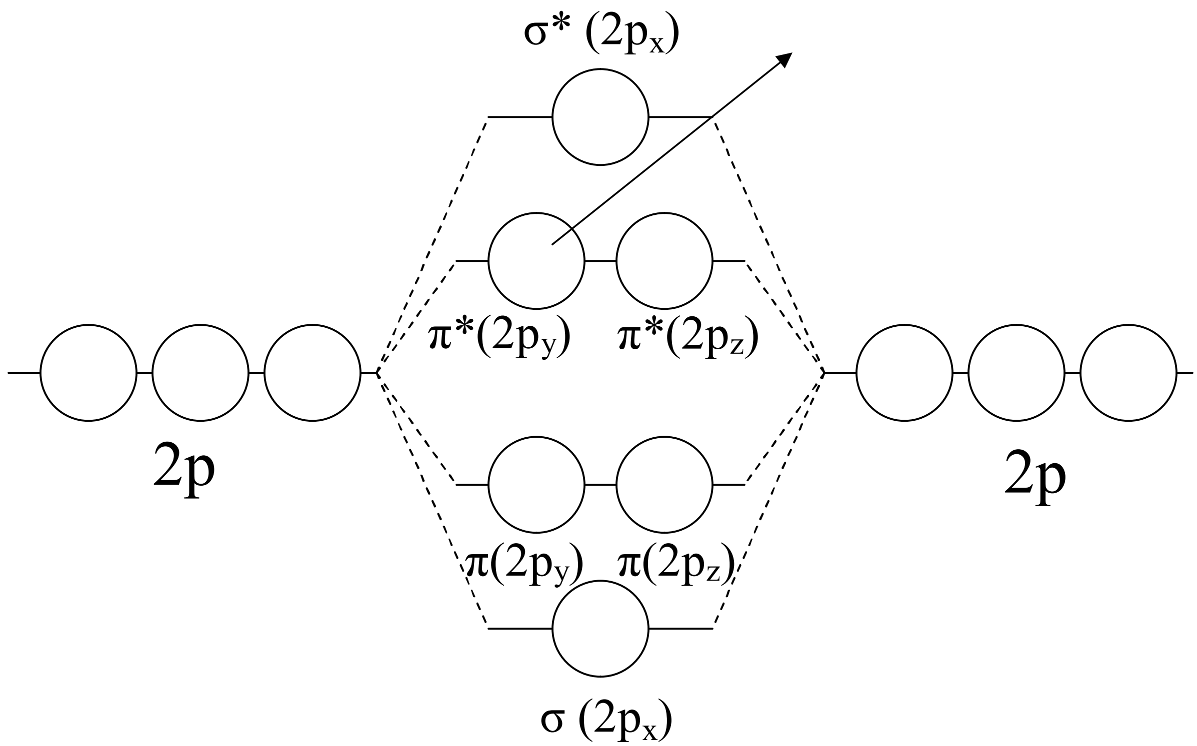
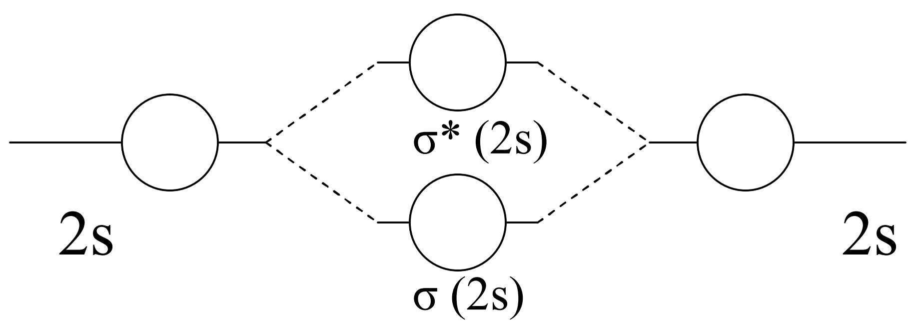


Energy (kcal/mole)
0
−80
−100
−200
−500
−1000
−2000
−5000
−10,000
−20,000
124
215
191
260
335
314
402
497
2s
1s
Li
$1s^22s$
Be
$1s^22s^2$
B
$1s^22s^22p^1$
C
$1s^22s^22p^2$
N
$1s^22s^22p^3$
O
$1s^22s^22p^4$
F
$1s^22s^22p^5$
Ne
$1s^22s^22p^6$

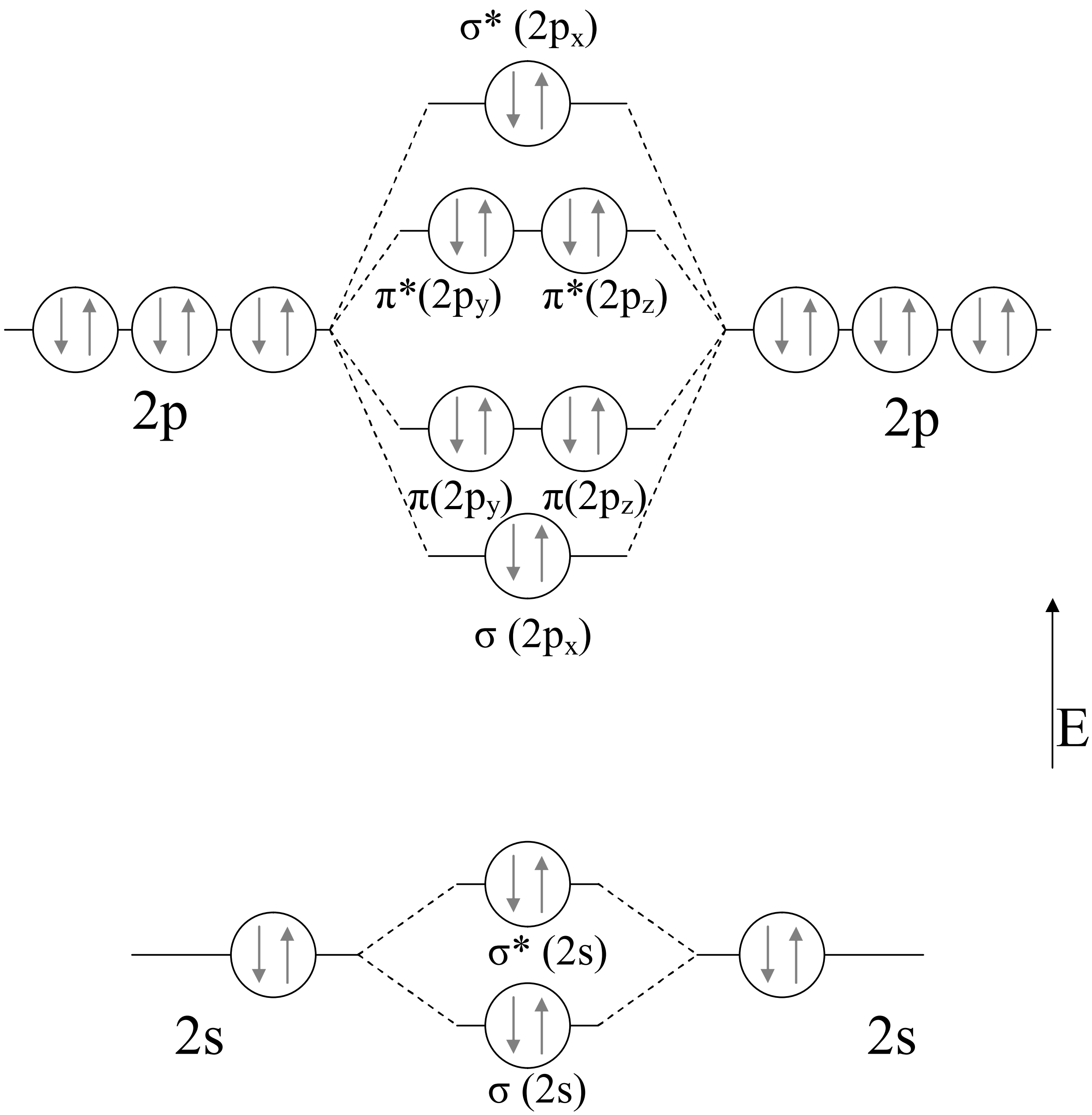


Combining atomic p orbitals
to molecular orbitals

Combining atomic orbitals to form molecular orbitals



Ne_2



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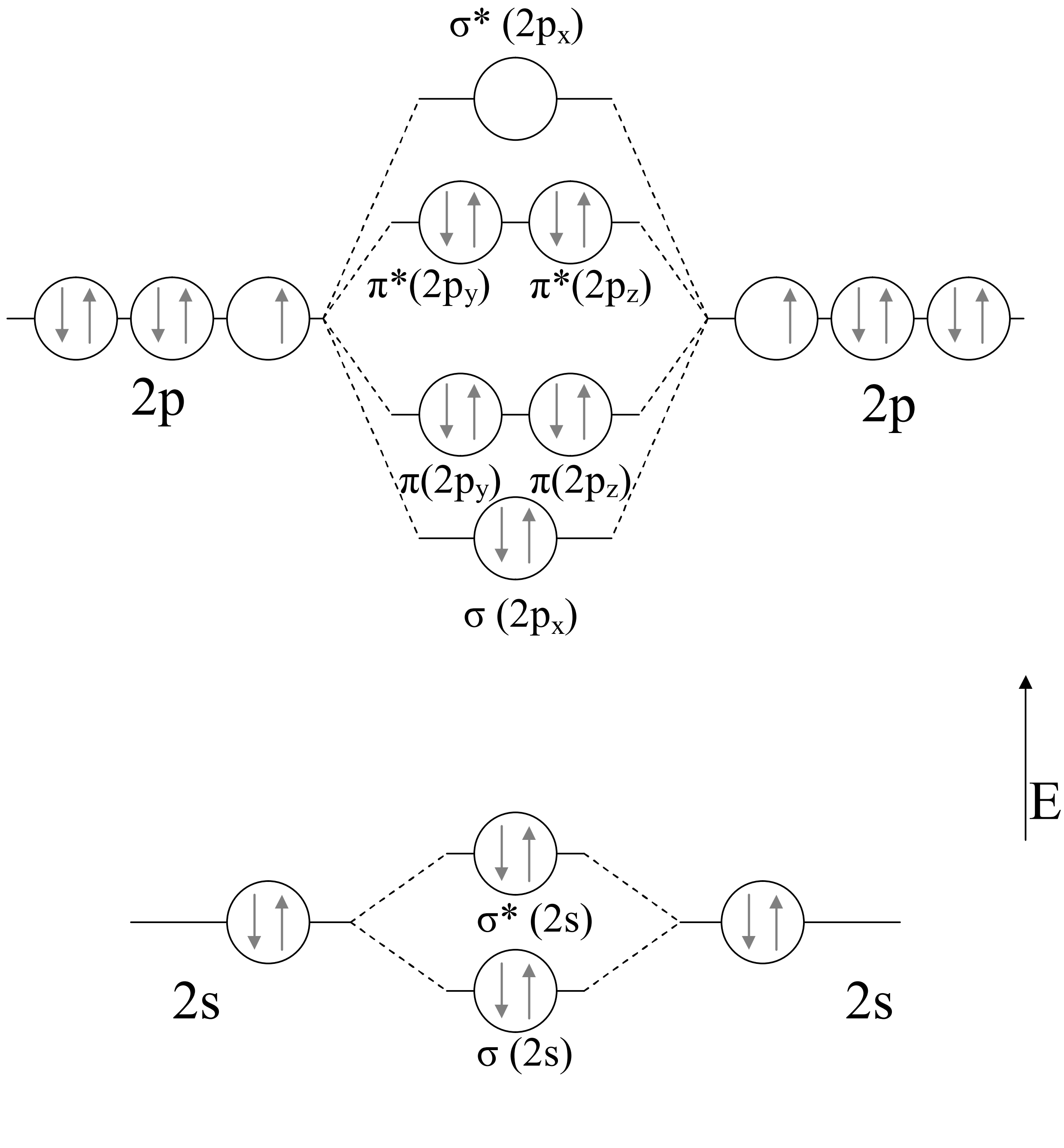
F_2



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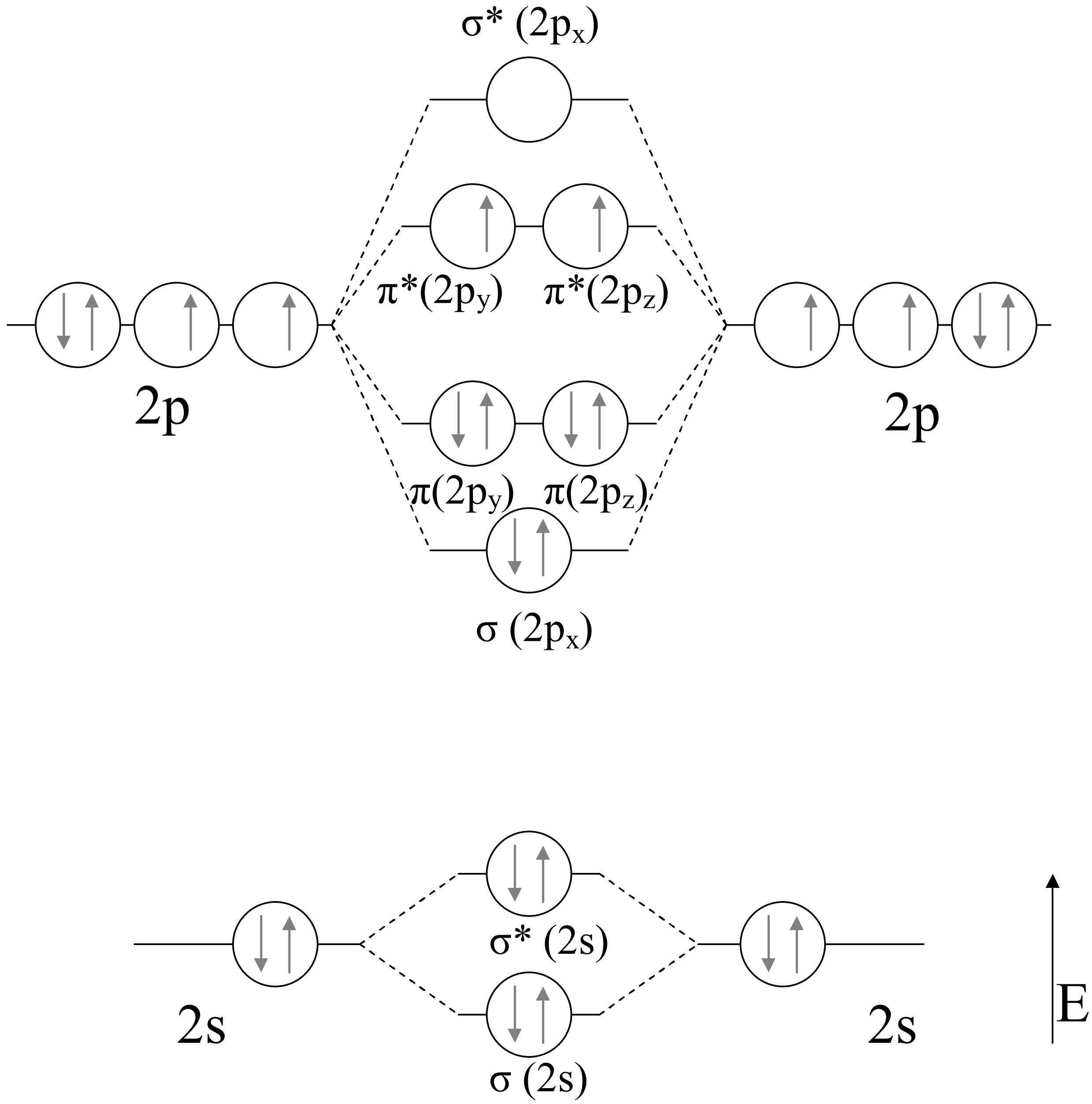
O_2



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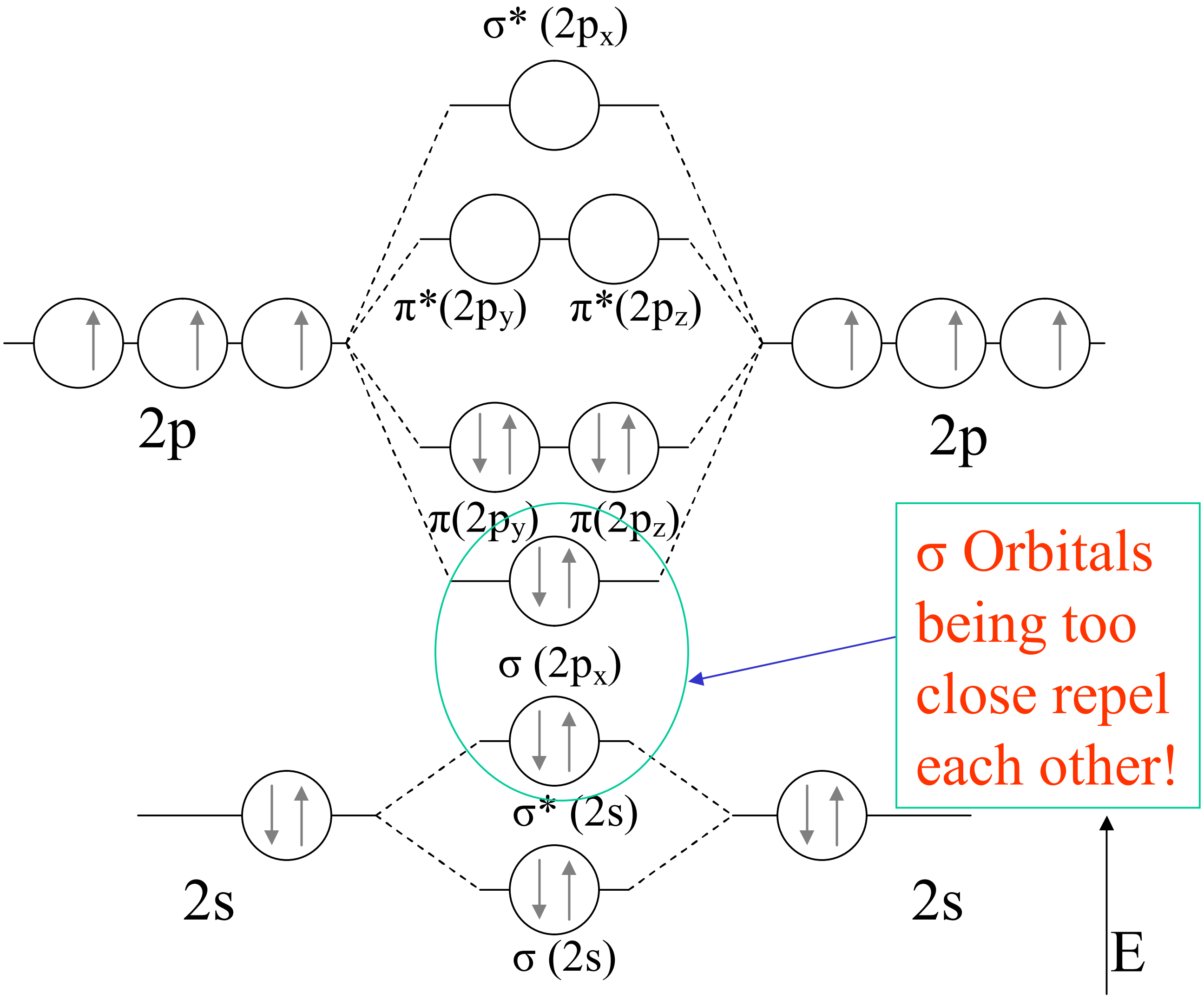
N_2



Before!!!

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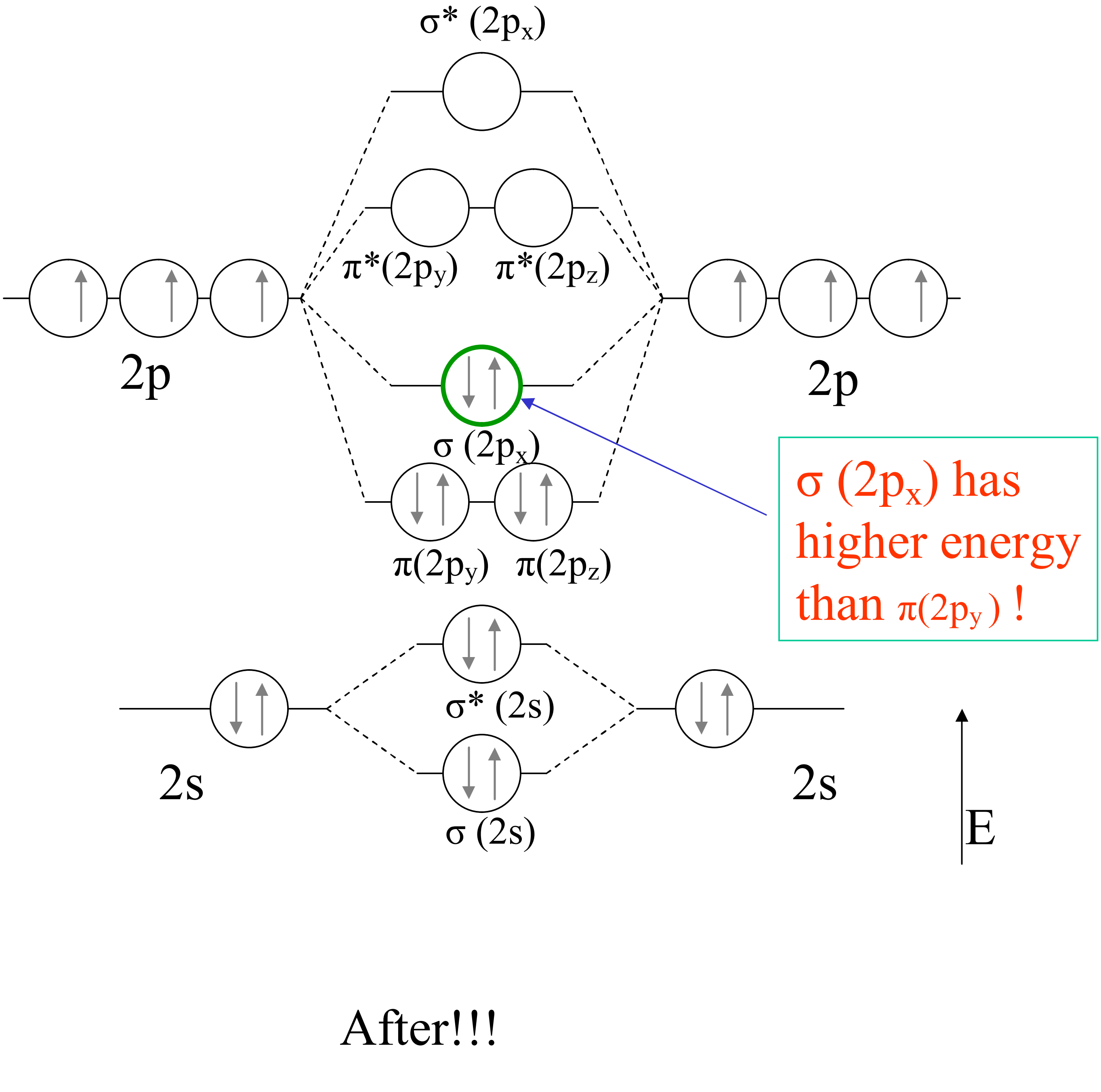
N_2



After!!!

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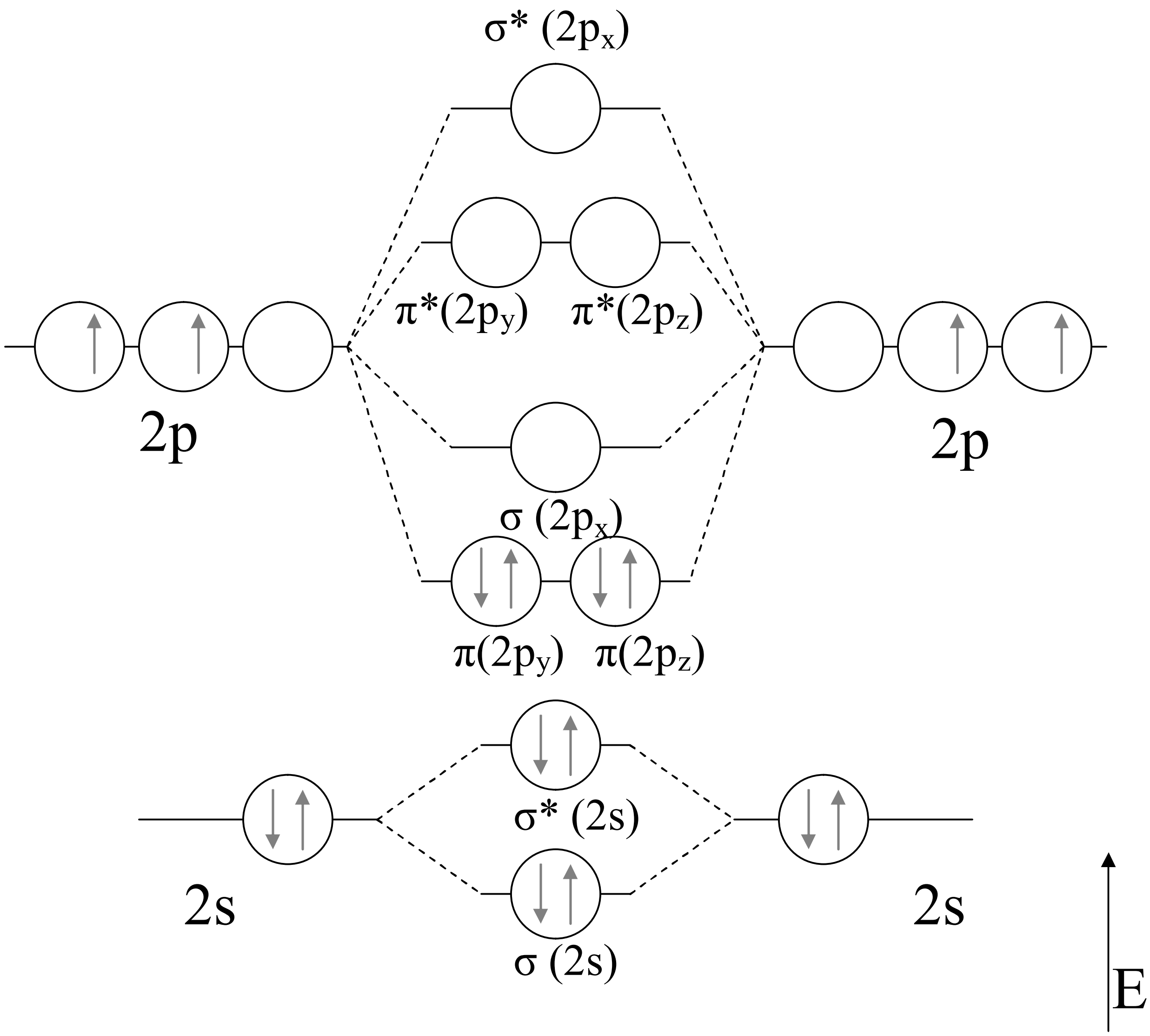
C_2



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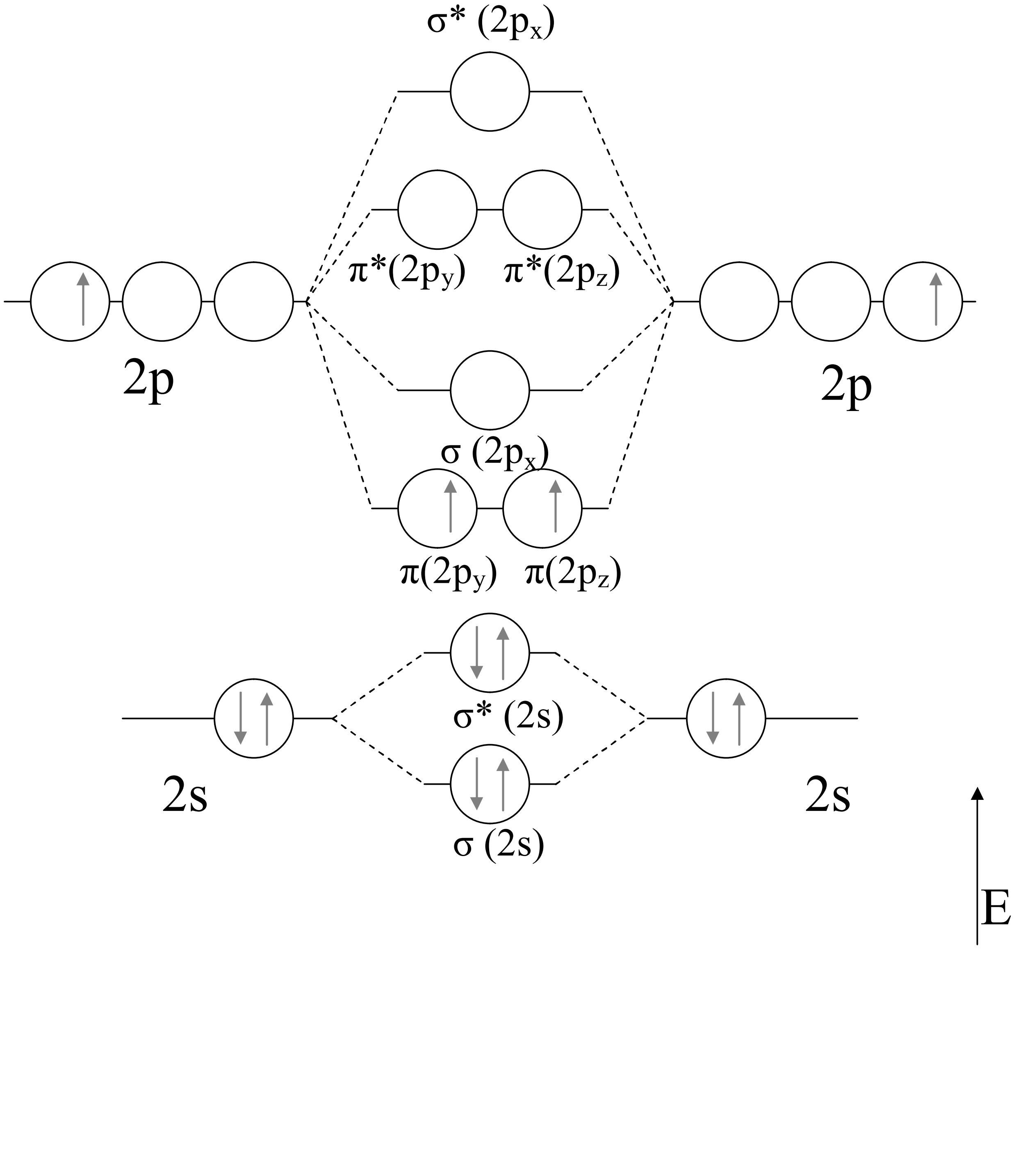
B_2



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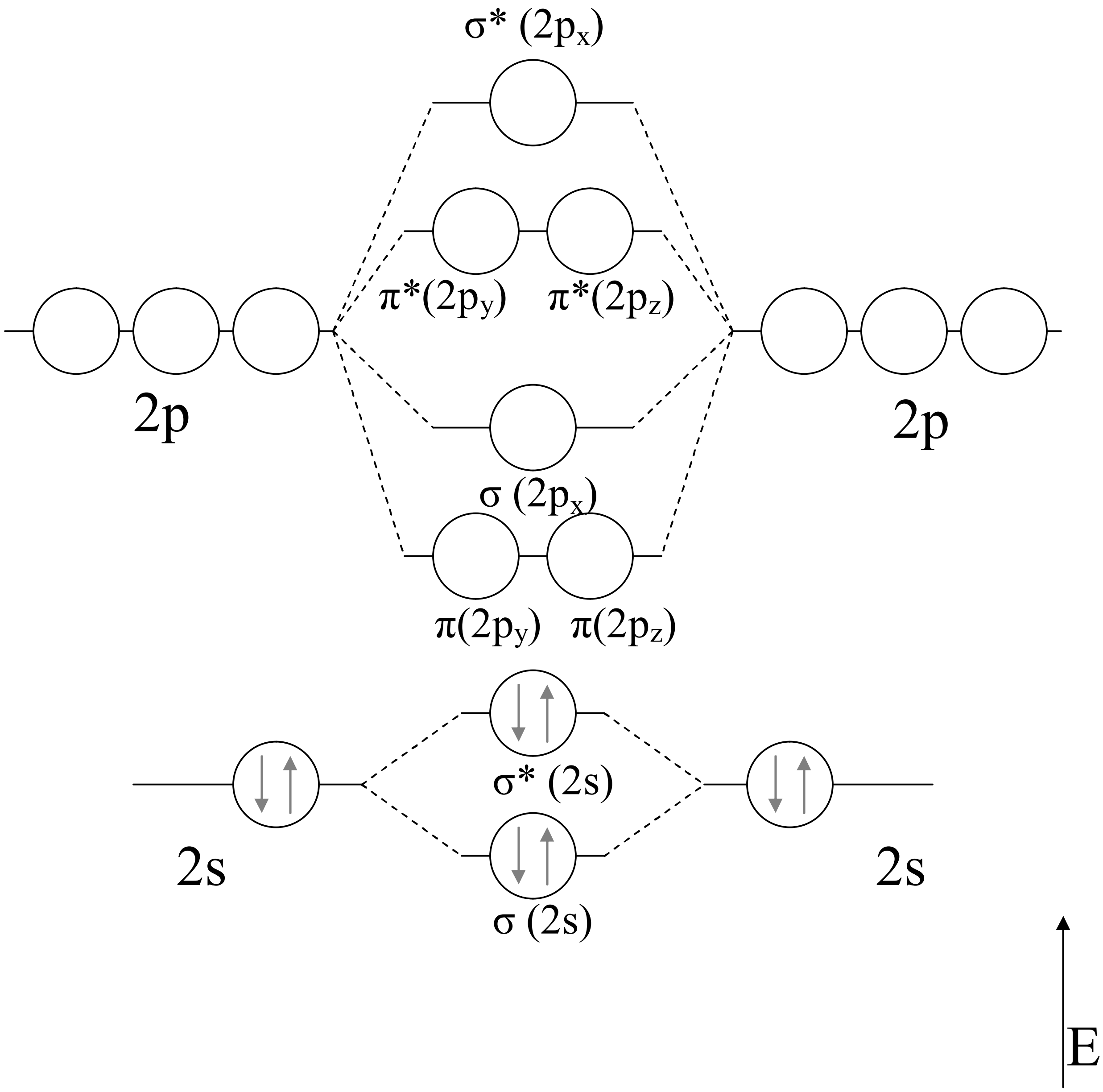
Be_2



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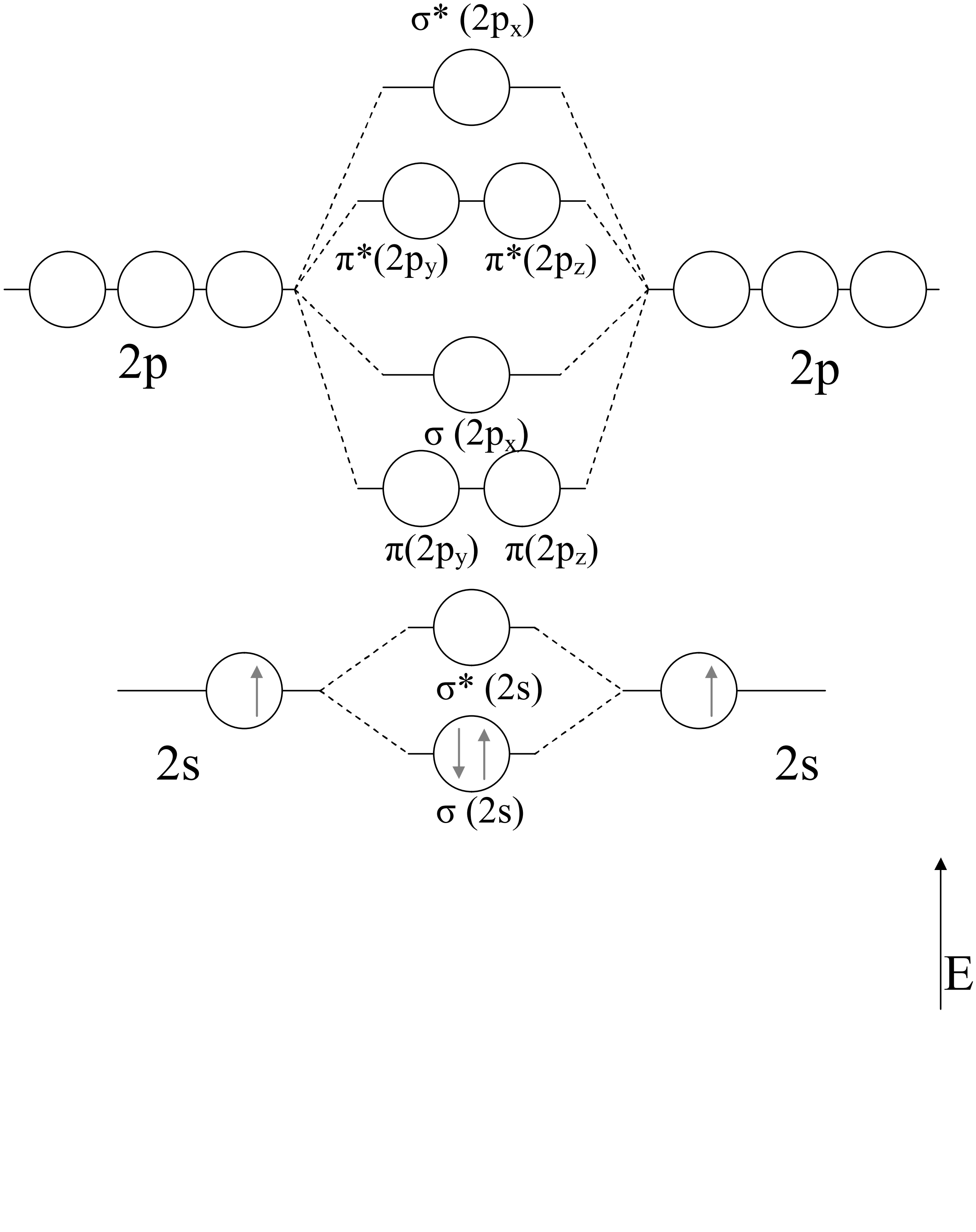
Li_2



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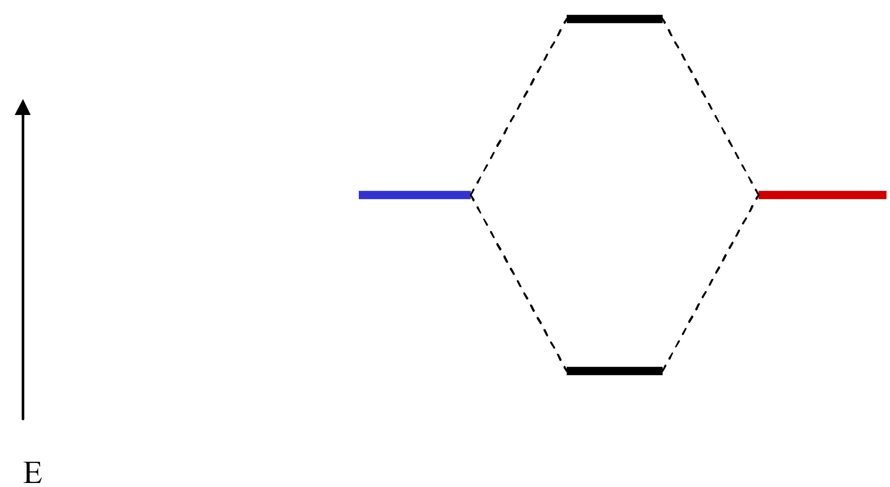
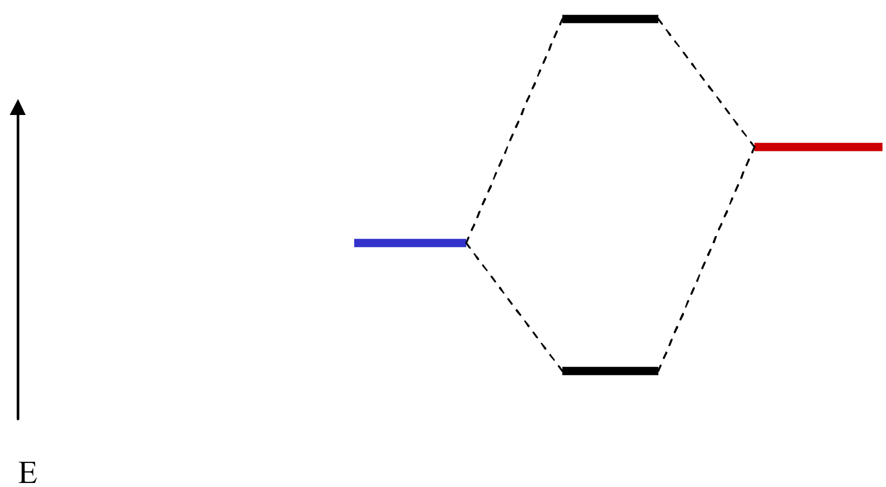
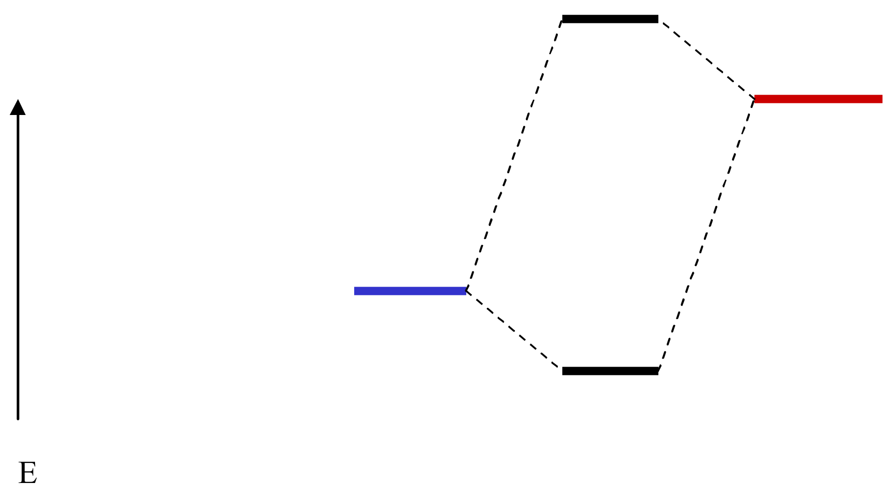
Perfect energy match!
Strongest bonding!



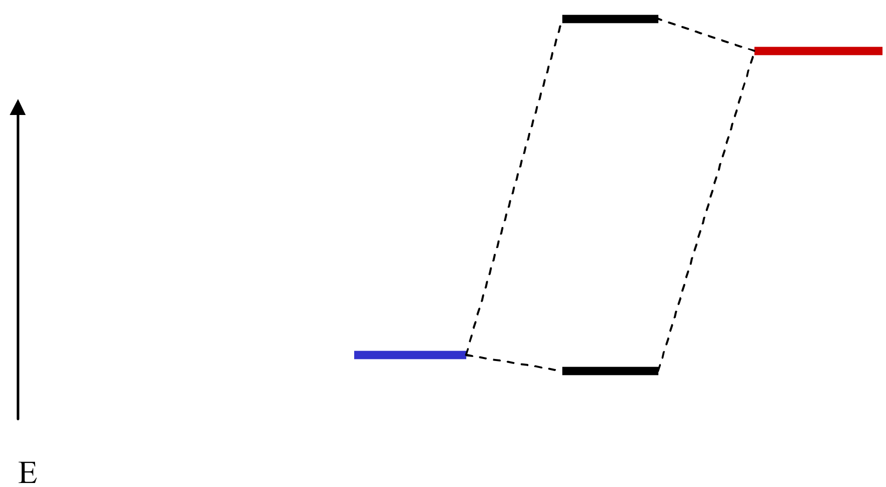
ok energy match!
still good bonding!



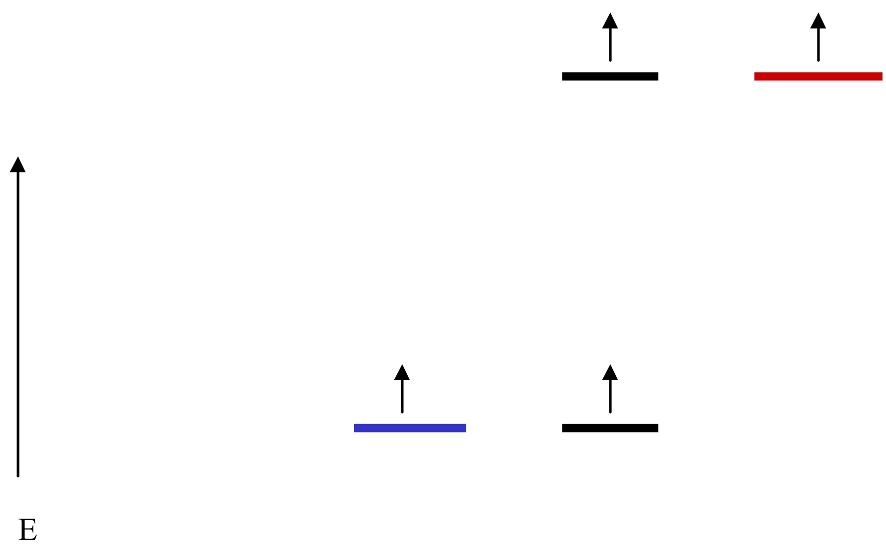
poor energy match!
weaker bonding!



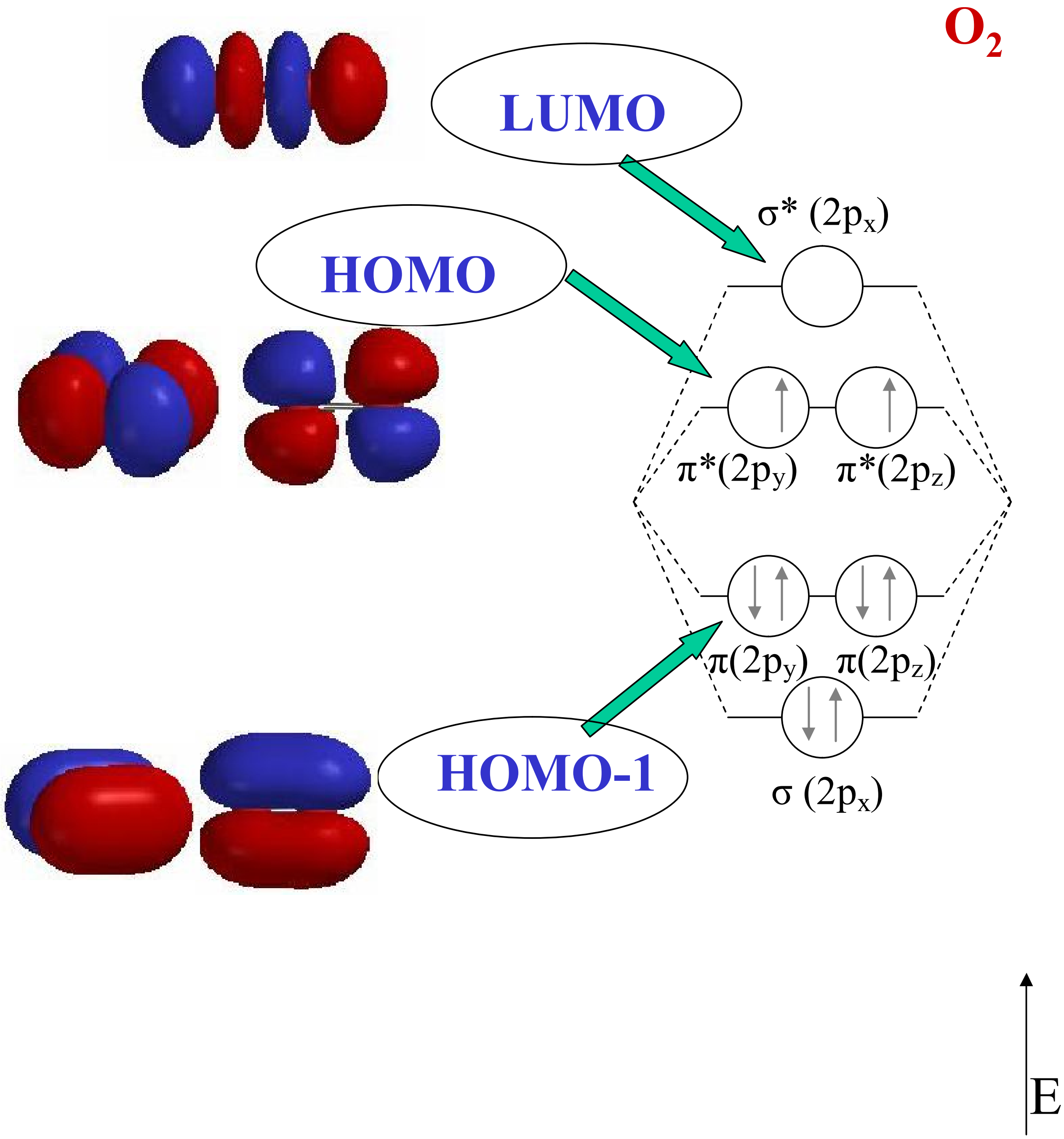
Badly matched!
very weak bonding!



no energy match!!
(non-bonding electrons)



LUMO: Lowest Unoccupied MO
HOMO: Highest Occupied MO
SOMO: Singly-Occupied MO (free radicals)



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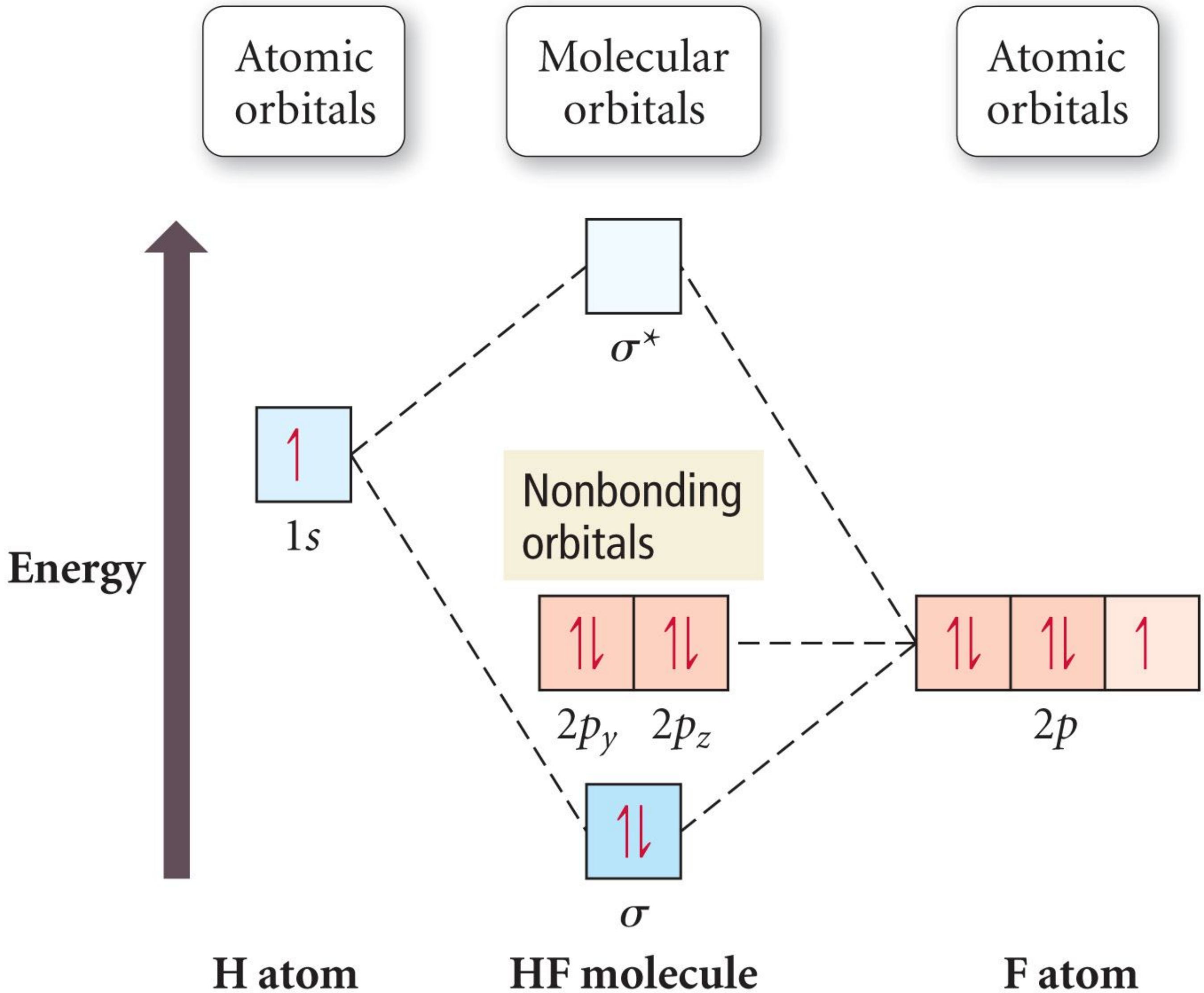

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1. Atomic orbitals are “wave containers”
2. An atom has infinite number of orbitals (n=1 to n=∞)
3. Electrons are the “wave contents”
4. Core electrons are complete orbitals that don’t contribute to bonding.
5. Valence electrons (orbitals) cause bonding.
6. A molecule is a combination of atoms with bonded (mixed) valence orbitals (electrons).
7. The extent of a covalent bond (mixing) is determined by the extent of match between energies of orbitals involved.
8. Electrons that fill antibonding MOs they weaken the bond!
9. An atom can hybridize its orbitals prior to mixing with another atom (ex. C_{sp3} – H_{1s}) to create a more stable bond (better overlap)
10. Orbital shape also matters for a strong overlap. (Py – Py and Pz – Pz versus Px – Px)