Molecular Orbital Theory

These slides may be downloaded at https://www.chemistrytuition.net/

Atomic Orbital Hybridisation

Atoms combine their atomic orbitals to produce hybrid orbitals

- sp^3 - Carbon in CH_4
- sp^2 – Boron in BF_3
- sp – Carbon in CO_2

We can think of the formation of new hybrid orbitals from the original atomic orbitals in terms of the wave functions of the atomic orbitals interfering to produce new hybrid orbitals – in a similar way that two waves on a pond will interfere with each other when they meet.

When atomic orbitals, whether hybridised or unhybridised combine to produce a chemical bond, they will also interfere with each other to produce molecular orbitals, these are labelled using the terminology of sigma, pi or delta.

Molecular Orbitals – H_2

Consider two hydrogen atoms forming a covalent bond. They both have 1 electron in their 1s orbital. Atomic hybridisation is unnecessary.

There are two possible outcomes when these two atomic orbitals interfere and produce molecular orbitals.

$1s^1$

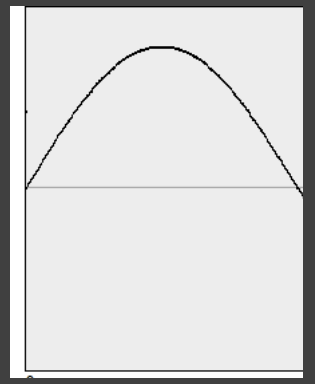
Hydrogen Atom A

$1s^1$

Hydrogen Atom B

Hydrogen
Atom A

+ phase

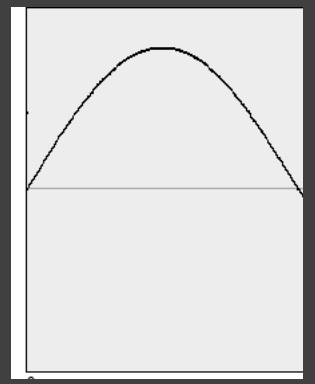


1s

Hydrogen
Atom B

+ phase

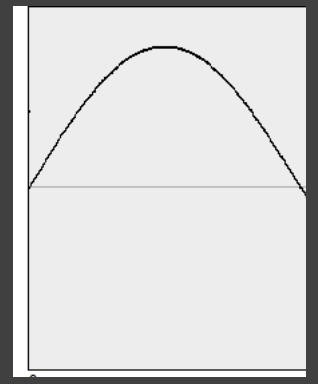
1s



Constructive interference

Hydrogen Atom A

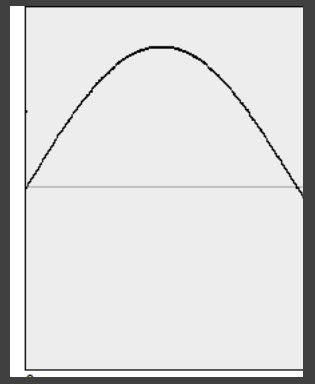
+ phase



1s

Hydrogen Atom B

+ phase

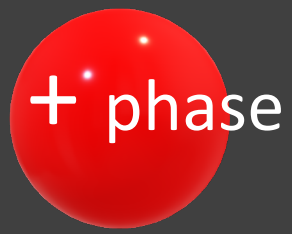


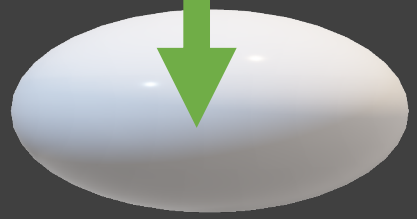
1s

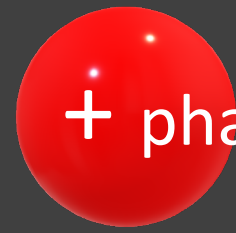
H_2 – a new bonding molecular orbital is formed

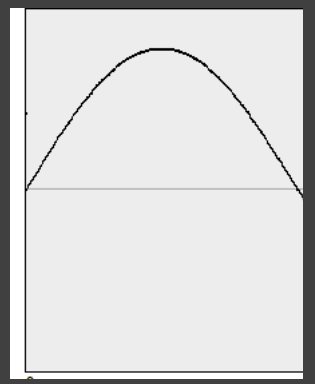
Hydrogen Atom A

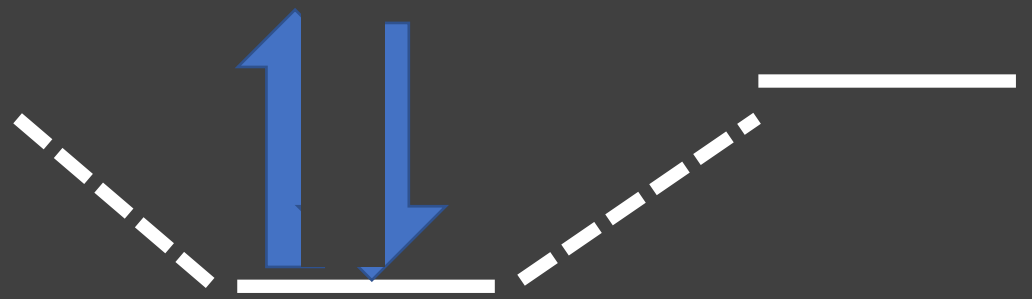
Hydrogen Atom B

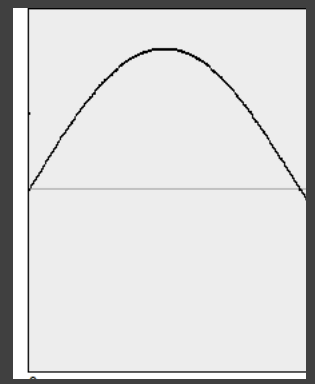












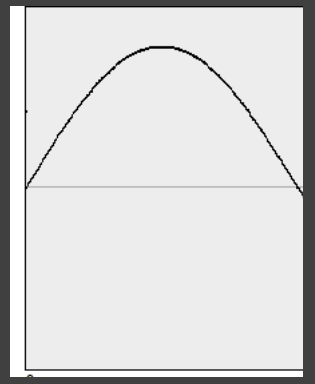
σ bonding orbital

Deconstructive interference

Hydrogen
Atom A

+ phase

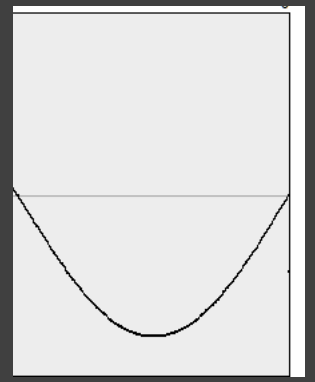
1s



Hydrogen
Atom B

- phase

1s

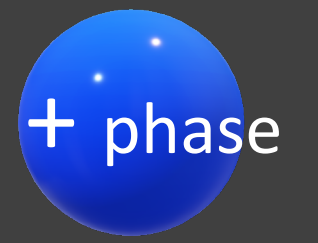


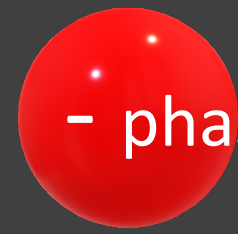
H_2 – a new antibonding molecular orbital is formed

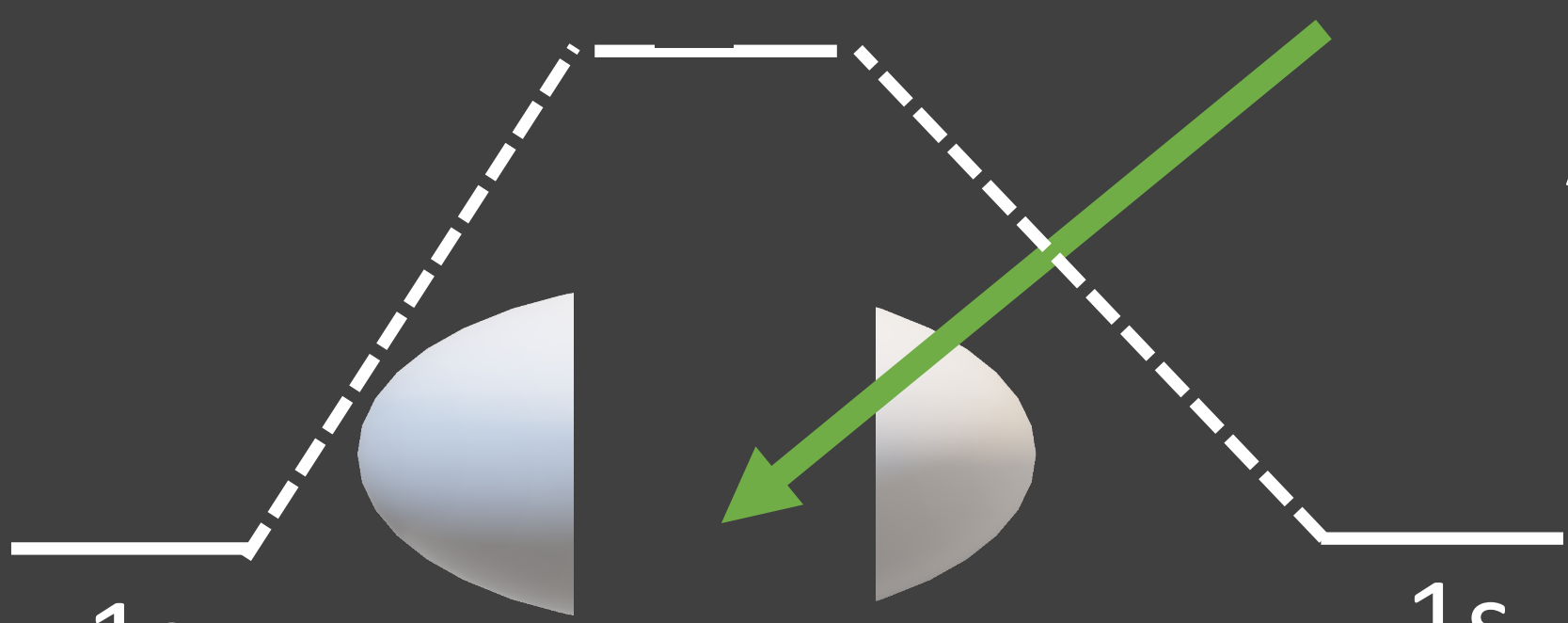
σ^* antibonding orbital

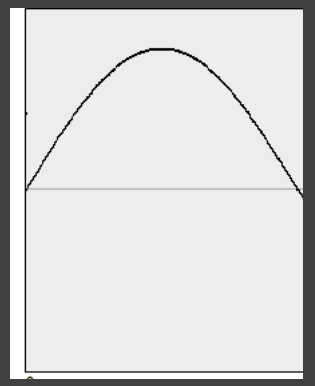
Hydrogen Atom A

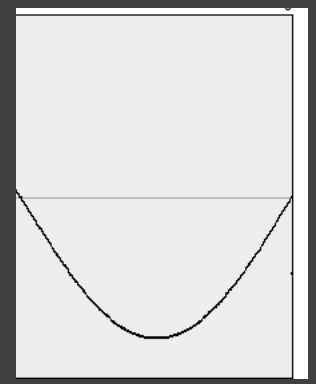
Hydrogen Atom B









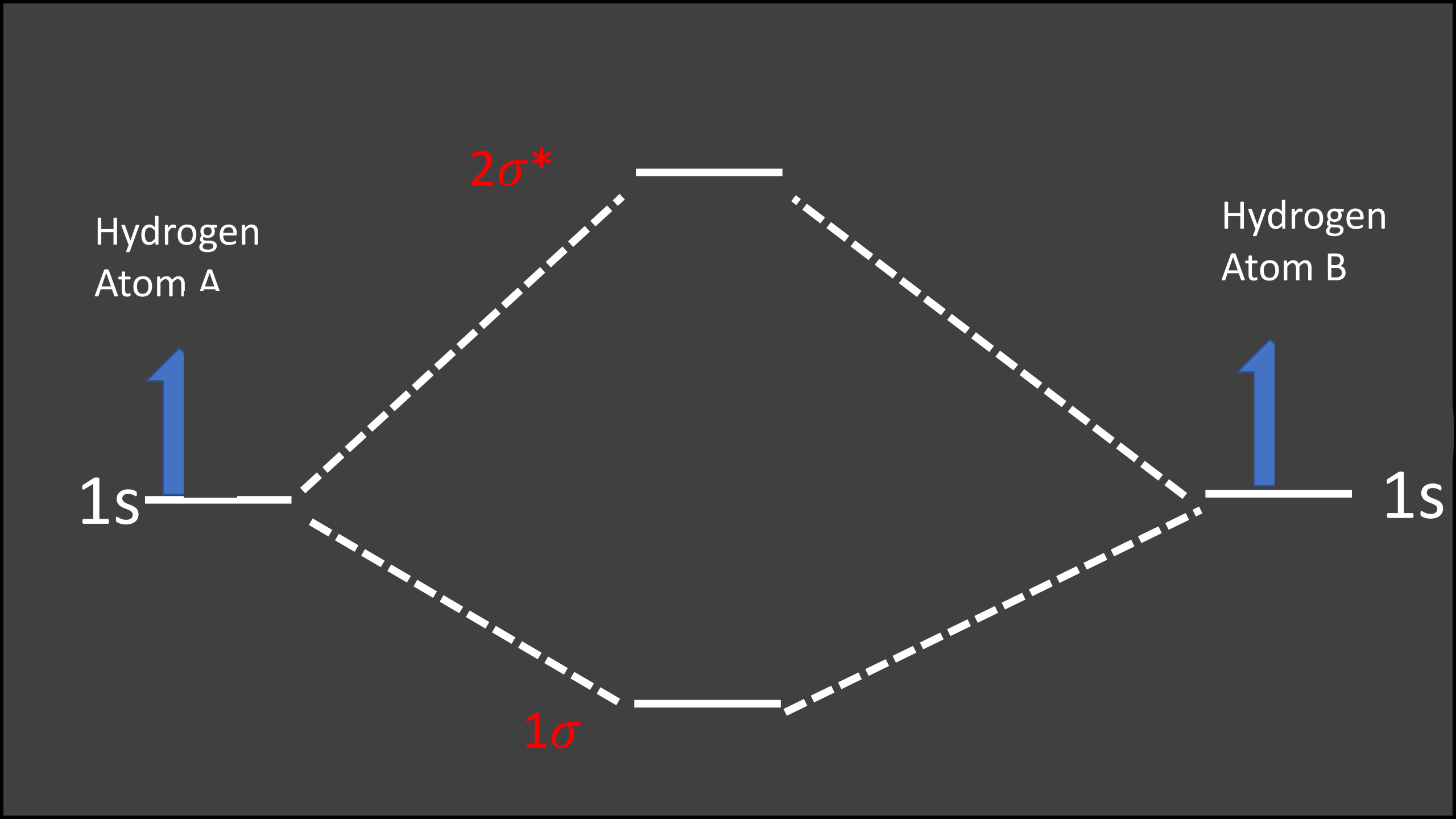


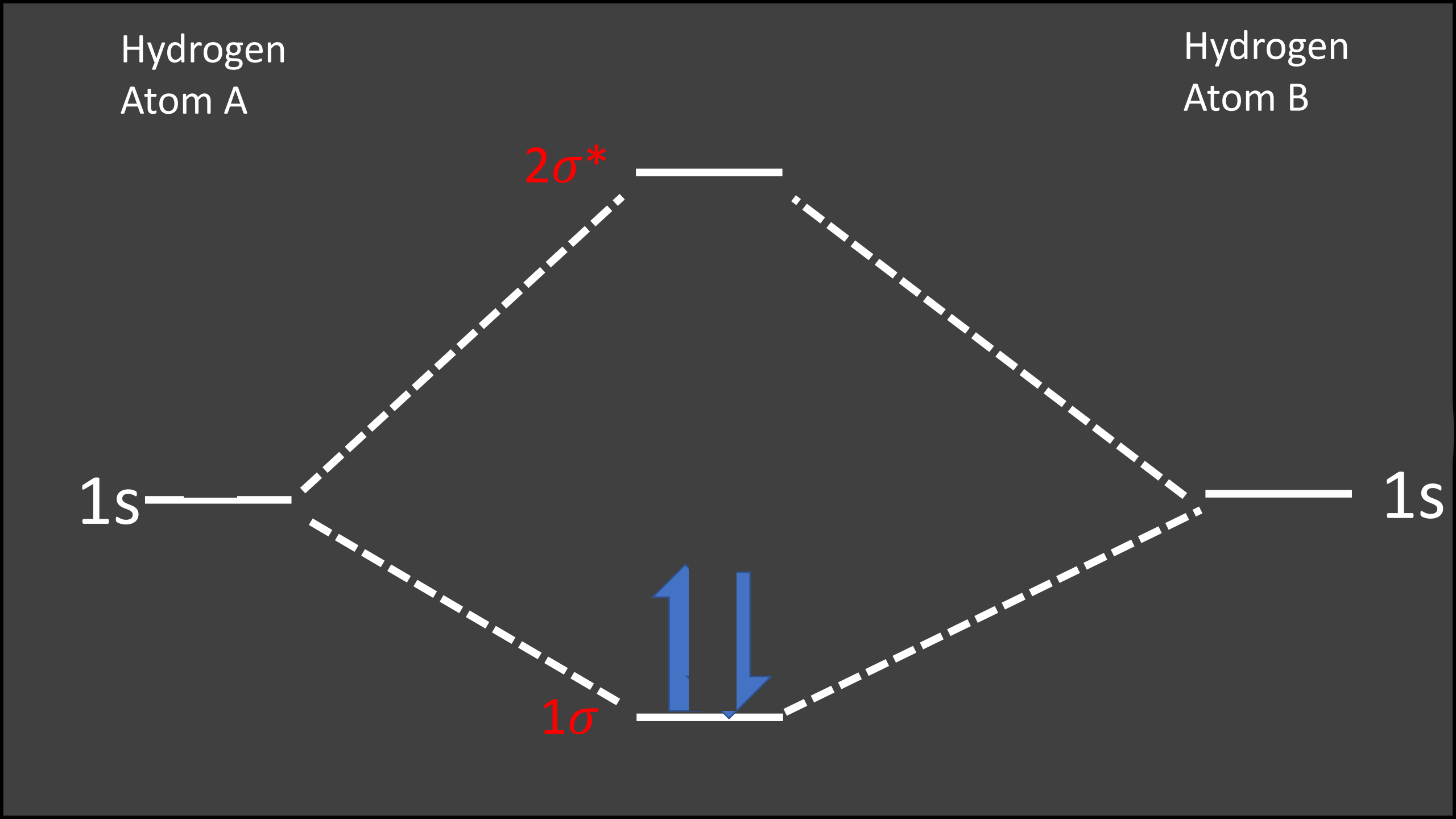
No electron density between the nuclei

When combining two atomic orbitals to form a bond there will always be two ways in which they can do this.

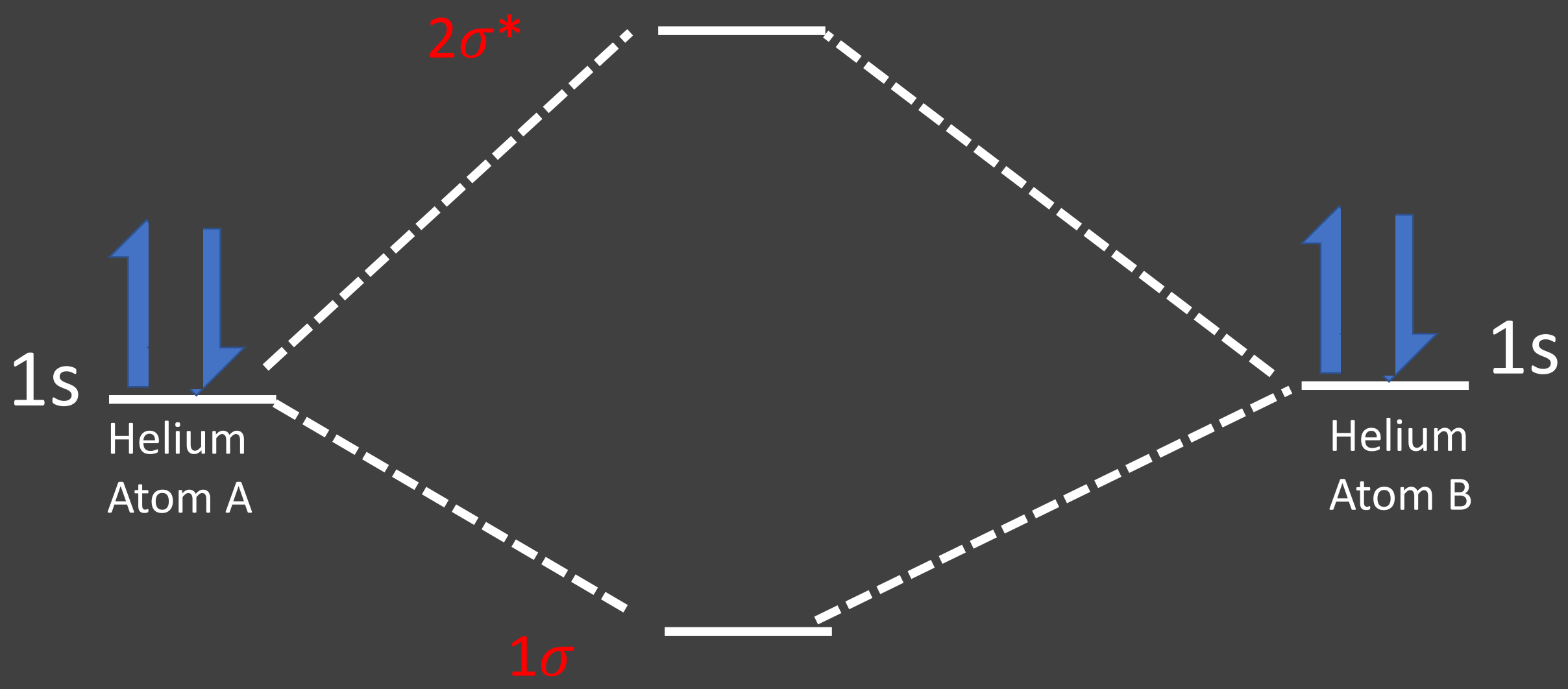
They can add such that there is constructive interference. This leads to bonding orbitals.

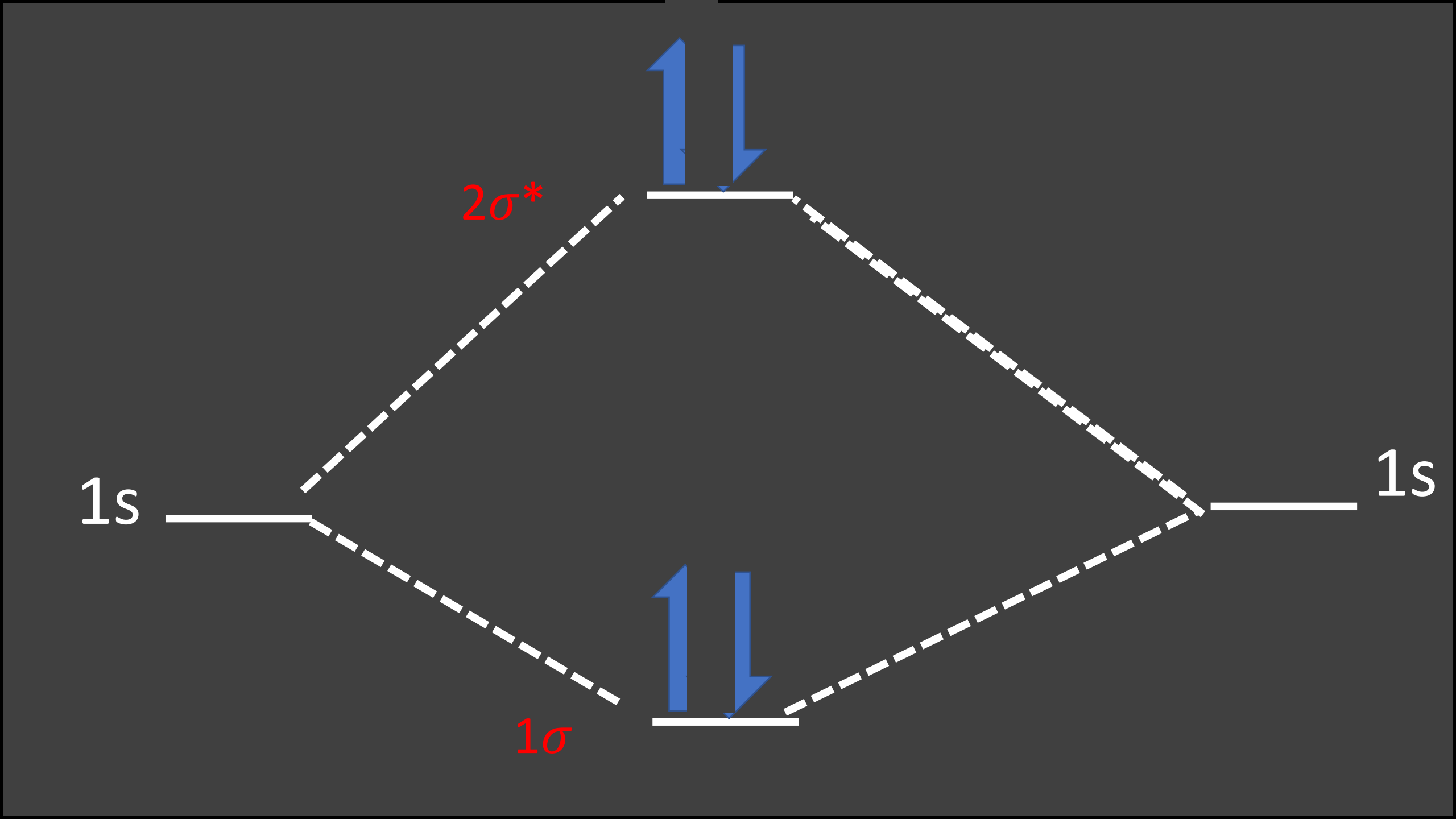
Or they can add up such that there is destructive interference. This leads to anti-bonding orbitals.

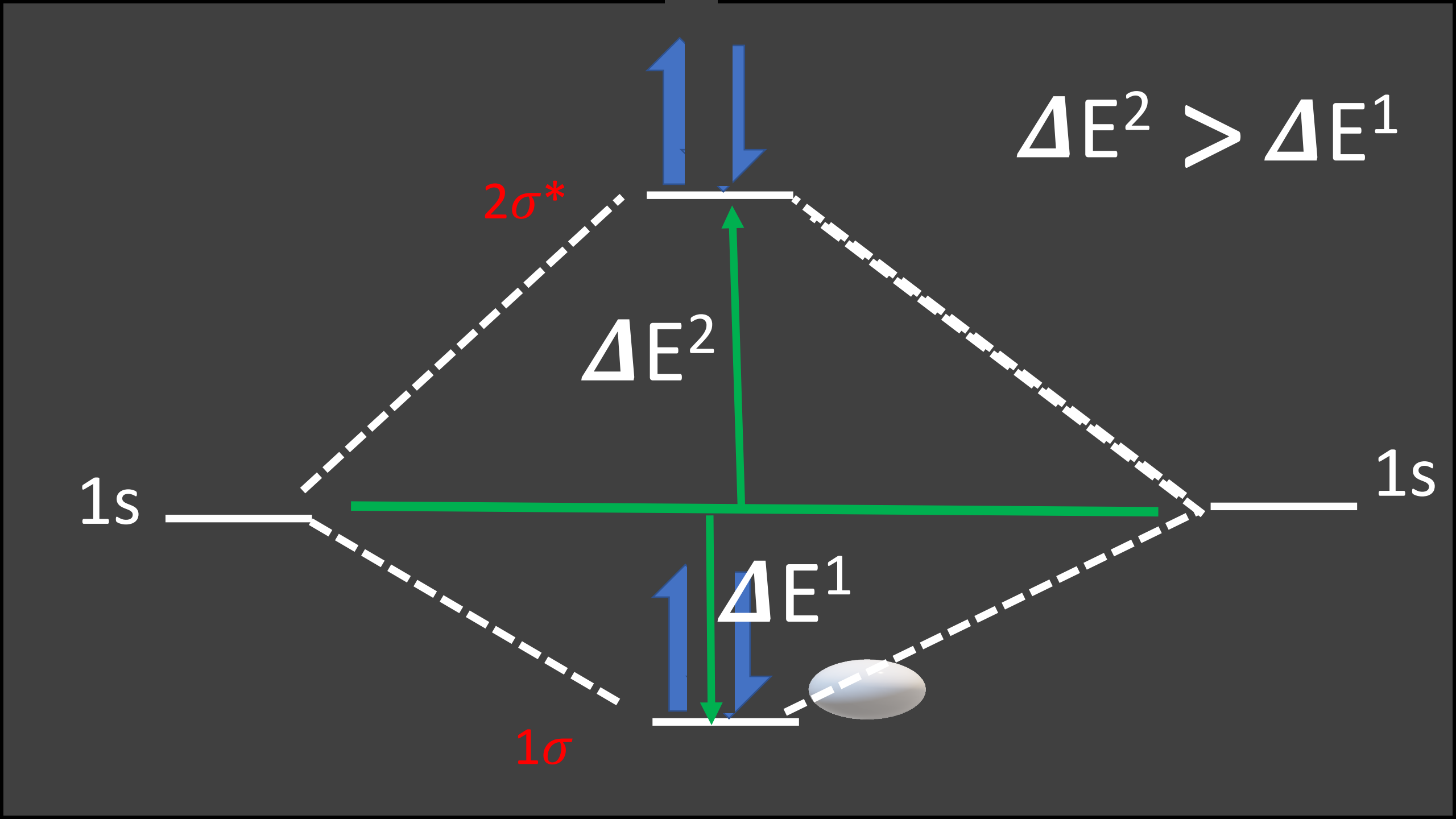

$2\sigma^*$
Hydrogen Atom A
Hydrogen Atom B
1
1
1s
1s
1σ


Hydrogen
Atom A
Hydrogen
Atom B
2σ*
1s
1s
1σ

What happens when two Helium atoms combine?


2σ*
1s
Helium
Atom A
1s
Helium
Atom B
1σ


2σ*
1s
1s
1σ


$\Delta E^2 > \Delta E^1$
$2\sigma^*$
ΔE^2
1s
1s
ΔE^1
1σ

Electronic Configurations

H_2

$2\sigma^*$

$1\sigma^2$

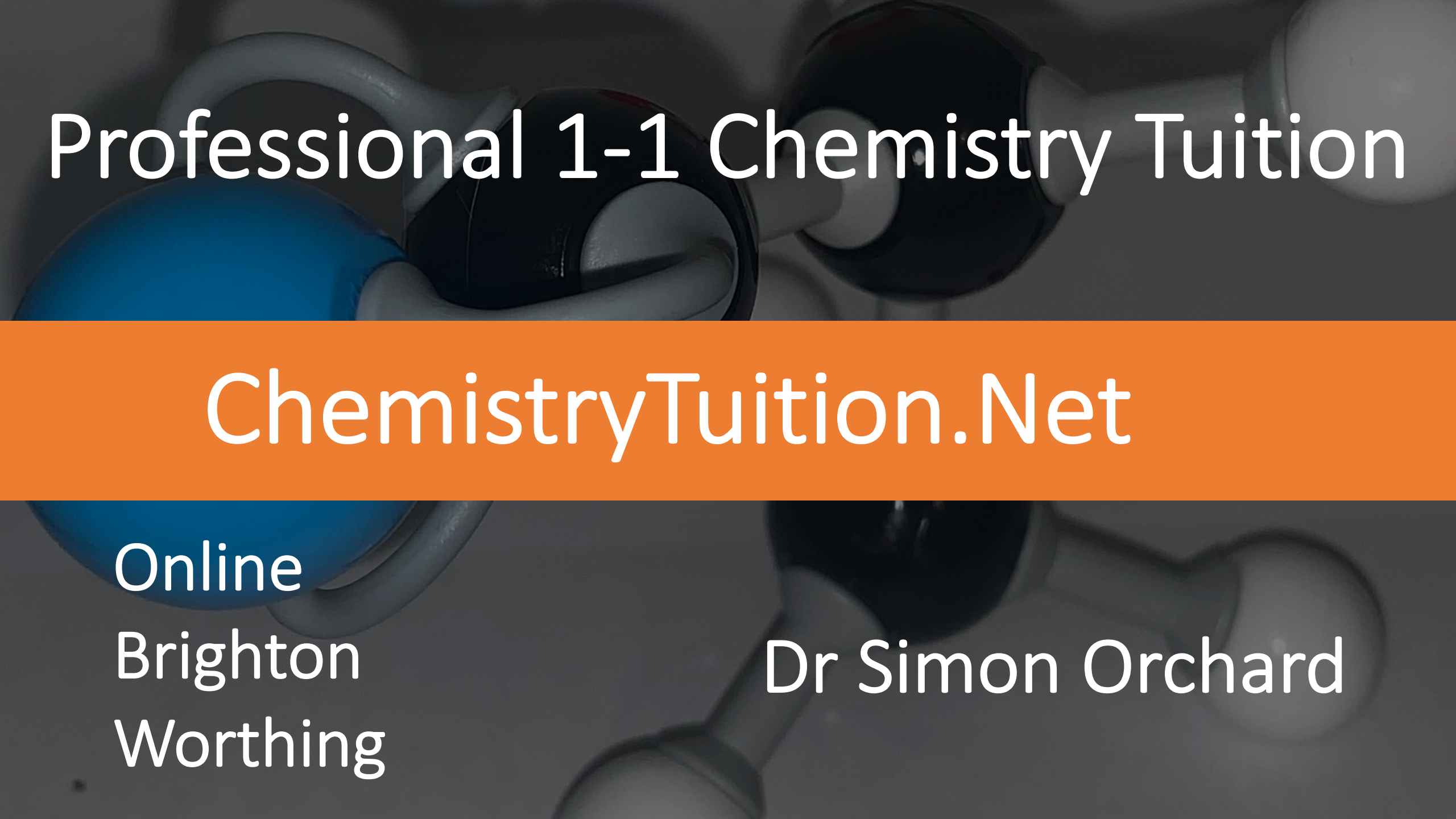
$1\sigma^2$

He_2

$2\sigma^{*2}$

$1\sigma^2$

$1\sigma^2\ 2\sigma^{*2}$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