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Supplementary Material

INTRODUCING AN ADDITIONAL CONCEPT IN CHEMICAL BONDING: HOW EFFECTIVELY CAN CHEMISTRY STUDENTS COMPREHEND CHARGE-SHIFT BONDING?

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Instructions for performing practical class

All quantum chemical calculations in this class were performed by means of the XMVB software package. In our case, we used computers with Linux operation system. The numerical data obtained from the XMVB output files were further processed in ESI.ods file which is also provided in the ESI.

In our case, to run the preint and xmvb one needs the following commands:

```
/opt/xmvb/bin/preint X.inp

/opt/xmvb/bin/xmvb X.xmi 1
```

where X.inp and X.xmi are the corresponding input files, which will be depicted below. Number 1 in the second command stands for the number of processors used in the calculation. Be cautious, in your case, the installation of XMVB might be in a different folder location. In that case /opt/xmvb/bin/ should be replaced with the right path. More information on installation and running the XMVB program can be found on the program webpage (http://www.xmvb.org/) or in a recent tutorial.

Description of chemical bonding in hydrogen molecule using valence bond (VB) theory

Within the VB theory framework, the bonding in H_2 molecule is described as a resonance between the three VB structures (one covalent and two ionic). This bonding description can be presented through the corresponding chemical structures, and this chemically reasonable sketch can be directly translated in the VB wavefunction, as shown in Fig. S1.

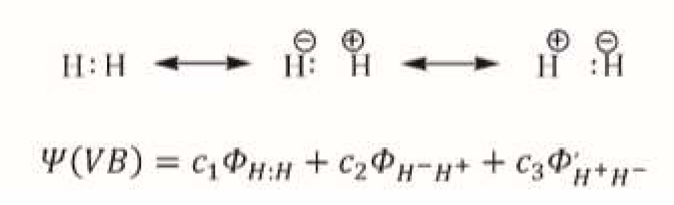


Fig. S1 The chemical bond between hydrogen atoms shown as a superposition of one covalent and two ionic VB structures and the corresponding VB wavefunction.

Our first task is to calculate the energy of the hydrogen molecule, whose VB wavefunction is depicted in Fig. S1. First, we calculate the energy of H_2 at the VBSCF/6-31G level. The needed XMVB input files, as well as all other input files, had been prepared before and all were collected in a single folder. Open VB input file H2-vb.xmi using any text editor (e.g., vi editor).

Table S1 XMVB input file for calculating the energy of the hydrogen molecule described by the wavefunction given in Fig. S1.

```
H2
 $ctrl
 itmax=5000 nstr=3 nao=2 nae=2 iscf=5 guess=unit
 nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
 $end
 $geo
 H 0.0 0.0 0.0
 H 0.0 0.0 0.741
 $end
 $str
 1 2
 1 1
 2 2
 $end
 $frag
 1*2
 spz 1   ; 1 H1
 spz 2   ; 2 H2
 $end
 $orb
 1 1
 1  ; s H 1
 2  ; s H 2
 $end
```

The $ctrl part defines the number of VB structures (nstr), active orbitals (nao), active electrons (nae), spin multiplicity (nmul), basis set (basis), and some other parameters, which are not described here in more detail. One of these is “orbtyp=hao frgtyp=sao” which specifies that we will use hybrid atomic orbitals in this calculation. In the $frag section, we specify how these hybrid orbitals will be obtained. In particular, for H_2 we allow s and p_z atomic orbital to mix and to give sp_z-hybrid orbitals. This means that the VB orbitals will be expressed in terms of the so-defined hybrid orbitals. The $orb section specifies VB orbitals, so VB orbital 1 is located on the first H

atom, and VB orbital 2 is located on the second H atom. Thus, the bond in H_2 will be described by the overlap of the two formally sp_z-hybrid orbitals. The $geo section contains the geometry of the molecule in cartesian coordinates. The distance between two hydrogen atoms corresponds to the experimentally determined value of 0.741 Å. There are two active electrons in the hydrogen molecule. The $str describes the VB structures used in this calculation:
"1 2" stands for covalent structure; two electrons with opposite spins occupy VB orbitals 1 and 2
"1 1" stands for ionic structure; both electrons occupy VB orbital 1
"2 2" stands for ionic structure; both electrons occupy VB orbital 2

From the working directory choose the command *Open in Terminal*. To start VB calculation, type the following command:

```
/xmvb_path/xmvb H2-vb.xmi 1
```

When the job is finished, in the working folder one can find the main output file: H2-vb.xmo. Open this file and find the line starting with "*Total Energy"* and copy the obtained energy into the .ods file in your folder. Check the values for the weights of VB structures in the same file, in the section named "*Weights of structures"*. In the hydrogen molecule, the covalent VB structure has the highest weight.

Now, we want to calculate the energy of the dominant VB structure. In the case of H_2, this is the covalent structure, so we proceed with calculation of E_{cov}. To accomplish this, use the input file H2cov-vb.xmi given below. The only difference from the first calculation is that this time in the $str section we specified only one structure.

Table S2 XMVB input file for calculating the energy of covalent structure for the hydrogen molecule.

```
H2
 $ctrl
 itmax=5000 nstr=1 nao=2 nae=2 iscf=5 guess=unit
 nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
 $end
 $geo
 H 0.0 0.0 0.0
 H 0.0 0.0 0.741
 $end
```

```
 $str
 1 2
 $end
 $frag
 1*2
 spz 1   ; 1 H1
 spz 2   ; 2 H2
 $end
 $orb
 1 1
 1  ; s H 1
 2  ; s H 2
 $end
```

Start this calculation by the following command:

```
/xmvb_path/xmvb H2cov-vb.xmi 1
```

In H2cov-vb.xmo find the energy value in the line starting with "*Total Energy*" and copy the value into the .ods file in your folder (E_{cov}).

The next step is to calculate the energy of the hydrogen molecule at the BOVB level. The input file is displayed in Table S3.

Table S3 XMVB input file for BOVB calculation for the hydrogen molecule.

```
H2
 $ctrl
 itmax=5000 nstr=3 nao=2 nae=2 iscf=2 guess=read bovb
 nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
 $end
 $geo
 H 0.0 0.0 0.0
 H 0.0 0.0 0.741
 $end
 $str
 1 2
 1 1
 2 2
 $end
 $frag
 1*2
 spz 1   ; 1 H1
 spz 2   ; 2 H2
```

```
$end
$orb
1 1
1  ; s H 1
2  ; s H 2
$end
```

This input file differs from the VBSCF input (Table S1) in the additional keyword *bovb*, and in *iscf* and *guess* options in the $ctrl section. Before running this job, we will use the obtained VBSCF orbitals as a guess in BOVB calculation. To do so, first we use this command:

```
cp H2-vb.orb H2-bovb.gus
```

Then, run VB calculation using the following command:

```
/xmvb_path/xmvb H2-bovb.xmi 1
```

In H2-bovb.xmo find the energy value and copy it into the .ods file in your folder.

In order to calculate the bond dissociation energy (BDE) we need to calculate the energy of the bond dissociation fragments, i.e. the energy of the hydrogen atom (E_H). At the dissociation distance VB wave function converged to the HF solution, so we will calculate the energy of an isolated H atom using the ROHF method. In the working folder, find the corresponding input file (H.inp).

Table S4 Input file for calculating the energy of the hydrogen atom at the ROHF/6-31G level of theory.

```
rohf 6-31g
0 2
H 0.0 0.0 0.0
```

Run calculation by the following command:

```
/xmvb_path/preint H.inp
```

In the output file H.log find the corresponding energy values and copy it to previously created .ods file. Now we have all the data to calculate the bond dissociation energy (BDE) and resonance energy (REcs).

Calculate the percentage contribution of the resonance energy (RE_{CS}) to the bond dissociation energy (BDE):

$$\%RE_{CS} = \frac{RE_{CS}}{BDE} \cdot 100 \tag{1}$$

Also, calculate the energy stabilization of the covalent structure (D_{cov}) as the difference between the BDE and RE_{CS}.

$$D_{cov} = BDE - RE_{CS} \tag{2}$$

While calculating the bond dissociation energy (BDE) and resonance energy (RE_{CS}) bear in mind that all energies are given in atomic units (Hartree per particle). It is practical to convert them to kJ mol^{-1} units.

Based on these values, classify the chemical bond in the hydrogen molecule.

Description of chemical bonding in fluorine molecule using valence bond (VB) theory

Within the VB theory framework, the bonding in F_2 molecule is described as a resonance between the three VB structures (one covalent and two ionic). This bonding description can be presented through the corresponding chemical structures, and this chemically reasonable sketch can be directly translated in the VB wavefunction, as shown in Fig. S2.

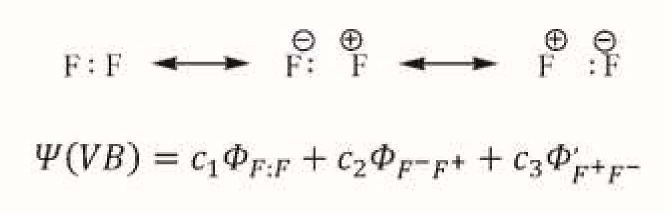


Fig. S2 The chemical bond between fluorine atoms shown as a superposition of one covalent and two ionic VB structures and the corresponding VB wavefunction.

Our first task is to calculate the energy of the fluorine molecule, whose VB wavefunction is given in Fig. S2. First, we calculate the energy of F_2 at the VBSCF/6-31G level. The needed XMVB input files, as well as all other input files, had been prepared before and all were collected in a single folder. Open VB input file F2-vb.xmi using any text editor (e.g., vi editor).

Table S5 XMVB input file for calculating the energy of the fluorine molecule described by the wavefunction given in Fig. S2.

```
F2
 $ctrl
 itmax=5000 nstr=3 nao=2 nae=2 iscf=5 guess=unit
 nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
 $end
 $geo
 F 0.0 0.0 0.0
 F 0.0 0.0 1.421
 $end
 $str
 1:8 9 10
 1:8 9 9
 1:8 10 10
 $end
 $frag
 1*6
 spz 1   ; 1 F1
 px 1    ; 2 F1
 py 1    ; 3 F1
 spz 2   ; 4 F2
 px 2    ; 5 F2
 py 2    ; 6 F2
 $end
 $orb
 1 1 1 1 1 1 1 1 1 1
 1  ; 1s F1
 4  ; 1s F2
 1  ; 2s F1
 4  ; 2s F2
 2  ; 2px F1
 5  ; 2px F2
 3 ; 2py F1
 6 ; 2py F2
 1  ; akt 2pz F1
 4 ; akt 2pz F2
 $end
```

The $ctrl part defines the number of VB structures (nstr), active orbitals (nao), active electrons (nae), spin multiplicity (nmul), basis set (basis), and some other parameters, which are not described here in more detail. One of these is “orbtyp=hao frgtyp=sao” which specifies that we will use hybrid atomic orbitals in this calculation. In the $frag section, we specify how these hybrid orbitals will be obtained. The $orb section specifies VB orbitals, so VB orbital 9 is located on the first F atom, and VB orbital 10 is located on the second F atom. Thus, the bond in F_2 will be described by the overlap of the two formally sp_z-hybrid orbitals. The $geo section contains the geometry of the molecule in cartesian coordinates. The distance between two fluorine atoms corresponds to the experimental value, 1.421 Å. There are two active electrons in the fluorine molecule. The $str describes the VB structures used in this calculation:

"1:8 9 10" stands for covalent structure; "1:8" means that inactive VB orbitals 1-8 are occupied by 2 electrons and two active electrons with opposite spins occupy VB orbitals 9 and 10

"1:8 9 9" stands for ionic structure; "1:8" means that inactive VB orbitals 1-8 are occupied by 2 electrons and both active electrons occupy VB orbital 9

"1:8 10 10" stands for ionic structure; "1:8" means that inactive VB orbitals 1-8 are occupied by 2 electrons and both active electrons occupy VB orbital 10.

From the working directory choose the command *Open in Terminal*. To start VB calculation, type the following command:

```
/xmvb_path/xmvb F2-vb.xmi 1
```

When the job is finished, in the working folder one can find the main output file: F2-vb.xmo. Open this file and find the line starting with "*Total Energy*" and copy the obtained energy into the .ods file in your folder. Check the values for the weights of VB structures in the same file, in the section named "*Weights of structures*". In fluorine molecule, the covalent VB structure has the highest weight.

Now, we want to calculate the energy of the dominant VB structure. In the case of F_2, this is the covalent structure, so we proceed with calculation of E_{cov}. To accomplish this, use the input file F2cov-vb.xmi given below. The only difference from the first calculation is that this time in the $str section we specified only one structure.

Table S6 XMVB input file for calculating the energy of covalent structure for the fluorine molecule.

```
F2
```

```
$ctrl
itmax=5000 nstr=1 nao=2 nae=2 iscf=5 guess=unit
nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
$end
$geo
F 0.0 0.0 0.0
F 0.0 0.0 1.421
$end
$str
1:8 9 10
$end
$frag
1*6
spz 1   ; 1 F1
px 1    ; 2 F1
py 1    ; 3 F1
spz 2   ; 4 F2
px 2    ; 5 F2
py 2    ; 6 F2
$end
$orb
1 1 1 1 1 1 1 1 1 1
1  ; 1s F1
4  ; 1s F2
1  ; 2s F1
4  ; 2s F2
2  ; 2px F1
5  ; 2px F2
3 ; 2py F1
6 ; 2py F2
1  ; akt 2pz F1
4 ; akt 2pz F2
$end
```

Start this calculation by the following command:

```
/xmvb_path/xmvb F2cov-vb.xmi 1
```

In F2cov-vb.xmo find the energy value in the line starting with "*Total Energy*" and copy the value into the .ods file in your folder (E_{cov}).

The next step is to calculate the energy of the hydrogen molecule at the BOVB level. The input file is displayed in Table S8.

Table S8 XMVB input file for BOVB calculation for the fluorine molecule.

```
F2
$ctrl
itmax=5000 nstr=1 nao=2 nae=2 iscf=2 guess=read bovb
nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
$end
$geo
F 0.0 0.0 0.0
F 0.0 0.0 1.421
$end
$str
1:8 9 10
$end
$frag
1*6
spz 1   ; 1 F1
px 1    ; 2 F1
py 1    ; 3 F1
spz 2   ; 4 F2
px 2    ; 5 F2
py 2    ; 6 F2
$end
$orb
1 1 1 1 1 1 1 1 1 1
1  ; 1s F1
4  ; 1s F2
1  ; 2s F1
4  ; 2s F2
2  ; 2px F1
5  ; 2px F2
3 ; 2py F1
6 ; 2py F2
1  ; akt 2pz F1
4 ; akt 2pz F2
$end
```

This input file differs from the VBSCF input (Table S1) in the additional keyword *bovb*, and in *iscf* and *guess* options in the $ctrl section. Before running this job, we will use the obtained VBSCF orbitals as a guess in BOVB calculation. To do so, first we use this command:

```
cp F2-vb.orb F2-bovb.gus
```

Then, run VB calculation using the following command:

```
/xmvb_path/xmvb F2-bovb.xmi 1
```

In F2-bovb.xmo find the energy value and copy it into the .ods file in your folder.

In order to calculate the bond dissociation energy (BDE) we need to calculate the energy of the bond dissociation fragments, i.e. the energy of the fluorine atom (E_F). At the dissociation distance VB wave function converged to the HF solution, so we will calculate the energy of an isolated F atom using the ROHF method. In the working folder, find the corresponding input file (F.inp).

Table S8 Input file for calculating the energy of the fluorine atom at the ROHF/6-31G level of theory.

```
rohf 6-31G
0 2
F 0.0 0.0 0.0
```

Run calculation by the following command:

```
/xmvb_path/preint F.inp
```

In the output file F.log find the corresponding energy values and copy it to previously created .ods file. Now we have all the data to calculate the bond dissociation energy (BDE) and resonance energy (REcs).

Calculate the percentage contribution of the resonance energy (RE_{CS}) to the bond dissociation energy (BDE) and the energy stabilization of the covalent structure (D_{cov}) using formulas (1) and (2).

Based on these values, classify the chemical bond in the fluorine molecule.

Description of chemical bonding in a sodium-chloride molecule using valence bond (VB) theory

Within the VB theory framework, the bonding in NaCl molecule is described as a resonance between the three VB structures (one covalent and two ionic). This bonding description can be presented through the corresponding chemical structures, and this chemically reasonable sketch can be directly translated in the VB wavefunction, as shown in Fig. S3.

$$\mathrm{Na{:}Cl} \longleftrightarrow \overset{\ominus}{\mathrm{Na}}{:}\ \overset{\oplus}{\mathrm{Cl}} \longleftrightarrow \overset{\oplus}{\mathrm{Na}}\ {:}\overset{\ominus}{\mathrm{Cl}}$$

$$\Psi(VB) = c_1\Phi_{Na:Cl} + c_2\Phi_{Na^-Cl^+} + c_3\Phi'_{Na^+Cl^-}$$

Fig. S3 The chemical bond between sodium and chlorine atoms shown as a superposition of one covalent and two ionic VB structures and the corresponding VB wavefunction.

Our first task is to calculate the energy of the sodium-chloride molecule, whose VB wavefunction is given in Fig. S3. First, we calculate the energy of NaCl at the VBSCF/6-31G level. The needed XMVB input files, as well as all other input files, had been prepared before and all were collected in a single folder. Open VB input file NaCl-vb.xmi using any text editor (e.g., vi editor).

Table S9 XMVB input file for calculating the energy of the sodium-chloride molecule described by the wavefunction given in Fig. S3.

```
NaCl
 $ctrl
 itmax=5000 nstr=2 nao=2 nae=2 iscf=5 guess=unit
 nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
 $end
 $geo
 Na 0.0 0.0 0.0
 Cl 0.0 0.0 2.361
 $end
 $str
 1:13 14 15
 1:13 15 15
 $end
 $frag
```

```
1*6
spz 1   ; 1 Na
px 1    ; 3 Na
py 1    ; 4 Na
spz 2   ; 2 Cl
px 2    ; 3 Cl
py 2    ; 4 Cl
$end
$orb
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
4  ; 1s Cl
1  ; 1s Na
4  ; 2s Cl
5  ; 2px Cl
6  ; 2py Cl
4  ; 2pz Cl
1  ; 2s Na
2  ; 2px Na
3  ; 2py Na
1  ; 2pz Na
4  ; 3s Cl
5  ; 3px Cl
6  ; 3py Cl
1  ; akt 2s Na
4  ; akt 3pz Cl
$end
```

The $ctrl part defines the number of VB structures (nstr), active orbitals (nao), active electrons (nae), spin multiplicity (nmul), basis set (basis), and some other parameters, which are not described here in more detail. One of these is “orbtyp=hao frgtyp=sao” which specifies that we will use hybrid atomic orbitals in this calculation. In the $frag section, we specify how these hybrid orbitals will be obtained. The $orb section specifies VB orbitals, so the active VB orbital 14 is located on the sodium atom, and active VB orbital 15 is located on the chlorine atom. Thus, the bond in NaCl will be described by the overlap of the two formally sp_z-hybrid orbitals. The $geo section contains the geometry of the molecule in cartesian coordinates. The distance between sodium and chlorine atoms corresponds to the experimental value, 2.361 Å. There are two active electrons in the sodium-chloride molecule. The $str describes the VB structures used in this calculation:

"1:13 14 15" stands for covalent structure; "1:13" means that inactive VB orbitals 1-13 are occupied by 2 electrons and two electrons with opposite spins occupy VB orbitals 14 and 15
"1:13 15 15" stands for ionic structure; "1:13" means that inactive VB orbitals 1-13 are occupied by 2 electrons and both active electrons occupy VB orbital 15
In the case of NaCl, the ionic structure where both electrons occupy VB orbital 14 in sodium atom was not included in this calculations, since it is expected that this structure will have very small weight.

From the working directory choose the command *Open in Terminal*. To start VB calculation, type the following command:

```
/xmvb_path/xmvb NaCl-vb.xmi 1
```

When the job is finished, in the working folder one can find the main output file: NaCl-vb.xmo. Open this file and find the line starting with "*Total Energy"* and copy the obtained energy into the .ods file in your folder. Check the values for the weights of VB structures in the same file, in the section named "*Weights of structures"*. In sodium-chloride molecule, ionic VB structure has the highest weight.

Now, we want to calculate the energy of the dominant VB structure. In the case of NaCl, this is the ionic structure, so we proceed with calculation of E_{ion}. To accomplish this, use the input file NaClion-vb.xmi given below. The only difference from the first calculation is that this time in the $str section we specified only one structure. Be cautious, since the VB orbital 14 in the previous calculation is now empty, this orbital is deleted, so now VB orbital 14 is orbital 15 from the previous calculation.

Table S10 XMVB input file for calculating the energy of ionic structure for the sodium-chloride molecule.

```
NaCl
 $ctrl
 itmax=5000 nstr=1 nao=1 nae=2 iscf=5 guess=unit
 nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
 $end
 $geo
 Na 0.0 0.0 0.0
 Cl 0.0 0.0 2.361
```

```
$end
$str
1:13 14 14
$end
$frag
1*6
spz 1   ; 1 Na
px 1    ; 3 Na
py 1    ; 4 Na
spz 2   ; 2 Cl
px 2    ; 3 Cl
py 2    ; 4 Cl
$end
$orb
1 1 1 1 1 1 1 1 1 1 1 1 1 1
4  ; 1s Cl
1  ; 1s Na
4  ; 2s Cl
5  ; 2px Cl
6  ; 2py Cl
4  ; 2pz Cl
1  ; 2s Na
2  ; 2px Na
3  ; 2py Na
1  ; 2pz Na
4  ; 3s Cl
5  ; 3px Cl
6  ; 3py Cl
4  ; akt 3pz Cl
$end
```

Start this calculation by the following command:

```
/xmvb_path/xmvb NaClion-vb.xmi 1
```

In NaClion-vb.xmo find the energy value in the line starting with "*Total Energy*" and copy the value into the .ods file in your folder (E_{ion}).

The next step is to calculate the energy of the hydrogen molecule at the BOVB level. The input file is displayed in Table S11.

Table S11 XMVB input file for BOVB calculation for the sodium-chloride molecule.

```
NaCl
```

```
$ctrl
itmax=5000 nstr=2 nao=2 nae=2 iscf=1 guess=read bovb
nmul=1 orbtyp=hao frgtyp=sao iprint=2 int=calc basis=6-31G
$end
$geo
Na 0.0 0.0 0.0
Cl 0.0 0.0 2.361
$end
$str
1:13 14 15
1:13 15 15
$end
$frag
1*6
spz 1   ; 1 Na
px 1    ; 3 Na
py 1    ; 4 Na
spz 2   ; 2 Cl
px 2    ; 3 Cl
py 2    ; 4 Cl
$end
$orb
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
4  ; 1s Cl
1  ; 1s Na
4  ; 2s Cl
5  ; 2px Cl
6  ; 2py Cl
4  ; 2pz Cl
1  ; 2s Na
2  ; 2px Na
3  ; 2py Na
1  ; 2pz Na
4  ; 3s Cl
5  ; 3px Cl
6  ; 3py Cl
1  ; akt 2s Na
4  ; akt 3pz Cl
$end
```

This input file differs from the VBSCF input (Table S1) in the additional keyword *bovb*, and in *iscf* and *guess* options in the $ctrl section. Before running this job, we will use the obtained VBSCF orbitals as a guess in BOVB calculation. To do so, first we use this command:

```
cp NaCl-vb.orb NaCl-bovb.gus
```

Then, run VB calculation using the following command:

```
/xmvb_path/xmvb NaCl-bovb.xmi 1
```

In NaCl-bovb.xmo find the energy value and copy it into the .ods file in your folder.

In order to calculate the bond dissociation energy (BDE) we need to calculate the energy of the bond dissociation fragments, i.e. energies of the sodium and chlorine atoms (E_{Na} and E_{Cl}). At the dissociation distance VB wave function converged to the HF solution, so we will calculate the energies of isolated Na and Cl atoms using the ROHF method. In the working folder, find the corresponding input files (Na.inp and Cl.inp).

Table S12 Input file for calculating the energy of the sodium atom at the ROHF/6-31G level of theory.

```
rohf 6-31g
0 2
Na 0.0 0.0 0.0
```

Table S13 Input file for calculating the energy of the chlorine atom at the ROHF/6-31G level of theory.

```
rohf 6-31G
0 2
Cl 0.0 0.0 2.361
```

Run calculations by the following command

-for sodium atom

```
/xmvb_path/preint Na.inp
```

-for chlorine atom

```
/xmvb_path/preint Cl.inp
```

In output files Na.log and Cl.log find corresponding energy values and copy them to previously created .ods file. Now we have all the data to calculate the bond dissociation energy (BDE) and resonance energy (REcs).

Calculate the percentage contribution of the resonance energy (RE_{CS}) to the bond dissociation energy (BDE) and the energy stabilization of the ionic structure (D_{ion}) using formulas (1) and (2).

Based on these values, classify the chemical bond in the sodium-chloride molecule.

Questionnaires (pre-test and post-test)

The pre-test questionnaire

1. Describe the formation of chemical bond between two hydrogen atoms ($_1H$) and define the type of chemical bonding in H_2.

2. Describe the formation of chemical bond between potassium ($_{19}K$) and fluorine ($_9F$) atoms and define the type of chemical bonding in KF.

3. Describe the formation of chemical bond between two fluorine ($_9F$) atoms and define the type of chemical bonding in F_2.

4. Define resonance hybrid.

5. Define resonance energy and bond dissociation energy.

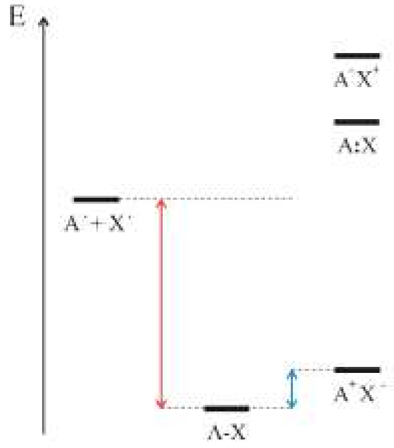
The post-test questionnaire

1. Describe the formation of chemical bond between two nitrogen atoms ($_7N$) and define the type of chemical bonding in N_2.

2. Describe the formation of chemical bond between magnesium ($_{12}Mg$) and chlorine atoms ($_{17}Cl$) and define the type of chemical bonding MgCl.

3. Describe the formation of chemical bond between two chlorine atoms ($_{17}Cl$) and define the type of chemical bonding in Cl_2.

4. What represents the energy difference marked in red and what in blue on the figure below?



5. Define charge-shift bonding (CSB).

6. Based on the values in table below (BDE - bond dissociation energy; RE – resonance energy) identify molecules from CSB family.

	BDE (kJ mol^{-1})	**RE (kJ mol^{-1})**
Li-Li	87.9	11.7
CH_3-F	415.1	296.6
Na^+Cl^-	332.6	42.3
Cl-Cl	164.4	203.8
Na-Na	54.4	0.0
CH_3-H	442.2	63.2
Na^+F^-	359.8	37.7
Br-Br	184.5	248.5
Li^+F^-	437.2	46.9

Table S14 Descriptive statistics (M-mean; SD-standard deviation) of selected (1-6) survey items

	Item	**2nd year undergraduate**		**MSc**		**PhD**	
		Mean	**SD**	**Mean**	**SD**	**Mean**	**SD**
1.	I am confident in my knowledge of chemical bond theory.	3.58	1.17	3.80	0.63	2.45	1.13
2.	I can distinguish a difference among types of chemical bonding.	4.38	0.64	4.60	0.52	4.45	0.52
3.	I consider my understanding of a covalent bond satisfactory.	4.23	0.95	4.30	0.67	4.18	0.60
4.	I consider my understanding of an ionic bond satisfactory.	4.00	1.17	4.20	0.63	4.27	0.65
5.	I was familiar with charge-shift bonding before this practical approach.	3.15	1.59	2.30	1.57	3.18	1.47
6.	Learning the theory of chemical bonding was challenging for me.	3.12	1.21	2.60	1.58	2.82	1.47

Table S15 Descriptive statistics (M-mean; SD-standard deviation) of selected (7-12) survey items

	Item	**2nd year undergraduate**		**MSc**		**PhD**	
		Mean	**SD**	**Mean**	**SD**	**Mean**	**SD**
7.	The practical approach helped me to understand better concept of chemical bonding.	4.65	0.56	4.50	0.85	4.55	0.69
8.	The practical approach helped me to understand better concept of covalent bonding.	4.58	0.58	4.60	0.70	4.64	0.50
9.	The practical approach helped me to understand better concept of ionic bonding.	4.50	0.58	4.40	1.07	4.64	0.50
10.	The practical approach helped me to understand better term bond dissociation energy.	4.50	0.65	4.60	0.70	4.64	0.50

11.	The practical approach helped me to understand better term resonance energy.	4.50	0.65	4.40	1.07	4.73	0.47
12.	The practical approach helped me to understand the concept of charge-shift bonding.	4.19	0.80	4.40	0.70	4.82	0.40

Table S16 Descriptive statistics (M-mean; SD-standard deviation) of selected (13-20) survey items

	Item	**2nd year undergraduate**		**MSc**		**PhD**	
		Mean	**SD**	**Mean**	**SD**	**Mean**	**SD**
13.	I find the practical training too hard and demanding.	2.00	1.33	1.40	0.52	2.18	1.47
14.	It was not hard for teacher and assistant to accompany the work of their students.	4.92	0.27	4.80	0.42	4.36	1.43
15.	The practical training contributes to my active participation during the practical class.	4.62	0.64	4.20	0.79	4.73	0.47
16.	I felt motivated during the practical exercise.	4.46	0.71	4.40	0.84	4.64	0.67
17.	I am looking forward to another similar activity.	4.46	0.76	4.60	0.70	4.45	1.04
18.	I think that the ICT competencies are important for every chemist	4.38	0.75	4.60	0.70	4.73	0.47
19.	During schooling, I had the chance to develop my ICT competencies.	3.62	1.36	3.80	1.14	3.91	1.14
20.	This practical training helped my ICT competencies to develop.	4.50	0.65	4.70	0.67	4.64	0.50