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

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The development of more modern and effective strategies for teaching chemical bonding theory is a key objective within the chemistry education community. A solid understanding of this concept is essential for comprehending a range of chemistry topics, including the physical and chemical properties of substances, chemical thermodynamics, and polymers – all of which play a vital role in real-world applications. Integrating valence bond (VB) theory, with its strong interpretative capabilities, into the teaching of chemical bonding through information and communication technologies (ICT) can help simplify complex ideas and enhance students comprehension. This paper presents a structured approach to explaining charge-shift bonding (CSB) within the VB theory framework by calculating the contributions of covalent and ionic VB structures, bond dissociation energy, and resonance energy. Additionally, it introduces unique teaching materials for university teachers and students, combining contemporary teaching tools with classical VB theory. The study involved 47 chemistry students, and the effectiveness of the practical training was assessed using three questionnaires, two knowledge tests (pre-test and post-test), and one survey. Results showed that MSc and PhD students were able to successfully grasp the fundamental concepts of CSB using the proposed approach, while undergraduate students encountered more difficulty. The practical class can serve as a valuable supplement to traditional upper-level instruction on chemical bonding, helping educators and students stay informed about more accurate and modern explanations of bonding in certain molecules.

Keywords: physical chemistry; chemical bonding; charge-shift bonding; upper-division undergraduate students; graduate education/research students

ВОВЕД ВО ДОПОЛНИТЕЛЕН КОНЦЕПТ НА ХЕМИСКО СВРЗУВАЊЕ: КОЛКУ ЕФИКАСНО МОЖАТ УЧЕНИЦИТЕ ПО ХЕМИЈА ДА ГО РАЗБЕРАТ СВРЗУВАЊЕТО СО ПРЕМЕСТУВАЊЕ НА ПОЛНЕЖ?

Развојот на поефективни и современи стратегии за предавање на теоријата за хемиско сврзување е една од главните цели на образовната заедница по хемија. Овој концепт е од суштинско значење за разбирање на разни други теми од хемијата, вклучувајќи ги физичките и хемиските својства на супстанции, хемиската термодинамика и полимерите – сите со клучна улога во секојдневниот живот. Интегрирањето на теоријата за валентни врски (VB) и нејзините интерпретативни способности во наставата за хемиско сврзување, во комбинација со информациските и комуникациските технологии (ICT), може да ја намали сложеноста и да овозможи подобро разбирање. Овој труд опишува постапка со цел да го објасни сврзувањето со преместување на полнеж (CSB) во рамките на VB-теоријата, преку пресметување на придонесите на ковалентните и јонските VB-структури, енергијата на дисоцијација на врската и енергијата на резонанцијата. Истовремено претставува и уникатен наставен материјал за универзитетски предавачи и студенти, комбинирајќи современи наставни алатки со пристапот на класичната теорија на валентни врски. Во студијата учествуваа 47 студенти по хемија, а можните ефекти од дизајнираната практична обука беа испитани преку три прашалници, два теста на знаење (пред-тест и пост-тест) и една анкета. Податоците собрани по практичниот час покажаа дека студентите на магистерски и докторски студии успешно ги разбираат основните концепти на CSB со користење на предложениот пристап, додека студентите на додипломски студии се соочија со потешкотии. Предложениот практичен час може да се вклучи како дополнителен материјал во традиционалната настава за концептот на хемиско сврзување на повисоко ниво, бидејќи универзитетската заедница, вклучително и студентите, треба да биде свесна за ново и попрецизно објаснување за поврзувањето во одредени молекули.

Клучни зборови: физичка хемија; хемиско сврзување; сврзување со преместување на полнеж; додипломски студенти од повисоките години; постдипломски студенти – образование/ истражување

1. INTRODUCTION

Chemical bonding is one of the central concepts in chemistry education and is fundamental to understanding nearly all topics in chemistry.[1–4] Students are introduced to this concept early in their academic chemistry education. A modern definition of chemical bonding has emerged through continuous scientific progress and has been shaped by numerous discoveries.[5–9]

When focusing on electron-pair bonding, it is widely accepted that there are two types of chemical bonds: ionic and covalent, which are distinguished based on the distribution of electrons within the bond.[10–13] Traditional approaches to teaching chemical bonding – especially in textbooks, emphasize these two types, while much less attention is given to other bonding types, such as metallic bonding.[14–16]

Chemistry students are typically taught two quantum-based approaches for describing a chemical bond: molecular orbital (MO) theory and valence bond (VB) theory. Continuous research within the VB framework over the past few decades has revealed a third class, known as charge-shift bonds (CSBs), in addition to covalent and ionic bonds.[17–20] Although this bond type was initially introduced through VB theory, the CSB concept has been supported by various interpretative approaches within MO theory.[19] More importantly, a recent study using many-electron probability density analysis, based on highly accurate wavefunctions, has provided further evidence for the CSB model.[21] A more detailed explanation of CSB is provided in the subsection, "2.2. Theoretical background and methods".

Students' understanding of bonding must be built incrementally by acquiring small pieces of knowledge and relating them to previously learned concepts.[22,23] Several studies have shown that chemistry students hold a wide range of conceptions of covalent and ionic bonding, some of which lack a solid scientific foundation.[24–29] Traditional teaching methods often fail to provide a deep understanding of chemical bonding and do not help students integrate their mental models into a coherent conceptual framework.[30–34]

Models play a crucial role in teaching chemical bonding due to the abstract nature of the concept.[35,36] In chemistry education, models are typically introduced through textbooks and teachers, and the way they are presented significantly influences students' comprehension.[37,38] While models are essential for facilitating understanding, they must be carefully selected and clearly explained, as poorly chosen or ambiguous models can lead to confusion.[39] Therefore, fostering a deep understanding of chemical bonding requires the use of a diverse range of models – from simple analogies to mathematical approximations.[35]

Because chemical bonding is an abstract concept, it requires the introduction of concrete elements to help students construct mental models for conceptual understanding. VB theory offers a variety of models that provide deeper insight into the nature of bonding, presenting visually intuitive wavefunctions expressed as linear combinations of chemically meaningful VB structures. Many foundational concepts in molecular chemistry – such as resonance (mesomerism), hybridization, and the arrow-pushing language used in reaction mechanisms, naturally arise from VB theory.

This study demonstrates how *ab initio* classical VB theory can serve as a valuable tool in chemical education, despite its historical underuse in this area. Integrating computational chemistry tools into the teaching of bonding can reduce conceptual complexity. These tools offer diverse pedagogical strategies and instructional technologies, enabling students to build mental models of chemical phenomena. Their application can enhance and extend students' knowledge while supporting constructivist learning, engagement, and student responsibility.[40–47]

2. EXPERIMENTAL SECTION

2.1. *Research aim and research questions*

Since the chemical bond plays a key role in describing the reactivity and physicochemical properties of molecules, it is important to develop a strong understanding of chemical bonds among students. Although the concept of the chemical bond has a long history, CSB is a relatively recent addition to the field. Initially introduced within the VB theory framework, the validity of the CSB concept has since been supported by numerous experimental and theoretical approaches.[21,48]

Research has shown that the CSB is a broad phenomenon occurring among a variety of elements across the periodic table. The CSB concept has enhanced our understanding of several bonding and reactivity challenges, including the inverted bond in [1.1.1]propellane and the unusual ionic chemistry of silicon in the condensed phase.[49,50] Additionally, CSB has proven useful in explaining cation-anion interface interactions in protic ionic liquids (PILs), where the CSB character correlates with key physicochemical properties such as melting point, conductivity, viscosity, and ionicity.[51] Furthermore, metal halides – promising candidates for optoelectronic applications due to their unique photophysical properties, also exhibit charge-shift bonding characteristics.[52,53] One of the central paradigms in bonding theory is that covalent bonding primarily arises from spin-exchange stabilization due to spin-pairing effects. However, numerous examples demonstrate that this is not always the case, providing the motivation for introducing the CSB model.[19] From a pedagogical perspective, the CSB concept offers a valuable framework for teaching chemical bonding and for explaining the various components of bonding energy. The authors argue that this makes a compelling case for incorporating the CSB concept into university level as a new concept in chemical bonding curricula.

This paper addresses the following research questions:

1. How efficiently can chemistry students understand the CSB concept?
2. What is the difference in understanding of CSB among students from different levels of study?
3. Based on students' attitudes does the proposed practical approach, grounded in ICT usage, contribute to an understanding of CSB?

While many studies have explored various aspects of teaching chemical bonding, to the best of the authors' knowledge, no formal proposals have been made for introducing students to CSB.[27,36,54] Developing instructional materials on chemical bonding that incorporates ICT is highly desirable, as it can enrich the curriculum and improve student outcomes. This paper presents a VB theory-based approach designed to make the concept of charge-shift bonding more accessible to students.

It is also important to note that several interpretative tools exist for localizing MO-based wavefunctions in a VB-like manner, such as the widely used Natural Bond Orbital (NBO) method.[55] However, NBO analysis has a limitation in describing CSB, as it does not clearly distinguish between covalent and ionic structures. Historically, VB methods were used by a small group of chemists, but in recent decades, VB theory has experienced a resurgence.[56] Advances in algorithms and the development of efficient new implementations[57] have made it possible to apply *ab initio* classical VB to a wide range of chemical problems.[58-61]

This paper proposes a practical teaching method based on *ab initio* VB calculations, which are rarely used in teaching practice. The proposed approach includes step-by-step instructions and is designed to be accessible to all teachers, not just experts in quantum chemistry. The applied methodology can be easily generalized and extended to a much wider group of molecules.

2.2. *Theoretical background and methods*

Although chemistry students learn about chemical bonding from a quantum chemical perspective – primarily through MO theory – when asked to describe a chemical bond, most students used terminology that originally emerged from the VB theory framework, such as Lewis structures and hybridization.[62] There are many prejudices regarding the perceived limitations of VB theory and a common belief that MO theory is inherently superior. However, already in 1930, it was demonstrated that both approaches are theoretically equivalent.[63,64] Today, with the availability of powerful computational resources, it is even easier to demonstrate that MO and VB are two equally valid frameworks for explaining chemical bonding.[65,66] This study employed the VB theory formalism to describe different bonding types and to introduce the concept of CSB.

The foundation of electron-pair bonding was established by Gilbert Newton Lewis more than a century ago.[8] Shortly thereafter, Heitler and London, in their seminal paper, provided the physical insight for Lewis's concept.[9] Pauling was the first to recognize that the wavefunction proposed by Heitler and London offered a rigorous quantum-mechanical description of the shared Lewis electron pair.[63] He further generalized the electron pair bond between atoms A–X as a superposition of covalent and ionic structures (Fig. 1).

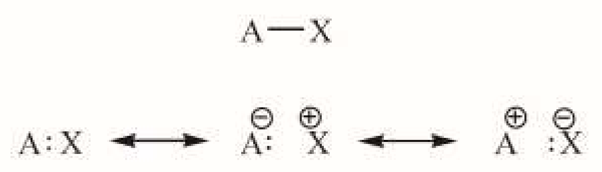

Fig. 1. The chemical bond between atoms (fragments) A and X shown as a superposition of one covalent and two ionic VB structures

The corresponding VB wavefunction describing Pauling's bonding scheme has the following form:

$$\Psi(VB)=c_1\Phi_{A:X}+c_2\Phi_{A^-X^+}+c_3\Phi_{A^+X^-} \qquad (1)$$

where the $\Psi(VB)$ represents the total VB wave function, $\Phi_{A:X}$ is a wavefunction of the covalent structure, where atoms A and X share an electron pair, $\Phi_{A^-X^+}$ and $\Phi_{A^+X^-}$ are wave functions of the ionic structures with both bonding electrons localized on A or X, respectively. The coefficients c_1, c_2 and c_3 reflect the contribution of each structure to the total VB wavefunction.

Figure 2 illustrates VB interaction diagrams for the three bonding types. According to Pauling's classification of electron-pair bonding, there are two primary bonding types: covalent and ionic. In covalent bonds, bonding arises mainly from spin-pairing stabilization, as described by the covalent structure. The bond dissociation energy (BDE) is primarily determined by the quantity D_{cov}, which corresponds to the energy stabilization of the covalent structure relative to the energy of the separate fragments in the homolytic dissociation limit.

Similarly, in ionic bonds, bonding primarily comes from the electrostatic stabilization between two oppositely charged fragments, as represented in one of ionic structures. As shown in Figure 2, Pauling's covalent-ionic bonding scheme downplays the role of resonance energy (RE_{CS}) in homopolar bonds, primarily due to the limited ability to accurately calculate such contributions in the 1930s.

It is worth noting that Pauling's original concept of electronegativity was based on covalent-ionic resonance energy. However, due to computational limitations of that era, it was assumed that the covalent-ionic resonance energy in homonuclear bonds could be neglected. The resonance energy RE_{CS} is also known as "charge-shift resonance energy" because it quantifies the electron-pair fluctuation resulting from covalent-ionic mixing (Fig. 1).

Thanks to advancements in computational power and systematic studies using modern VB methods in the 1990s, a third class of electron-pair bonding was identified under the name charge-shift bonding (CSB). In this bonding type, resonance energy is the dominant contributor to the overall bonding energy (Fig. 2c).

It has been recommended that a chemical bond should be classified as a CSB if the value of the RE_{CS} is greater than 50 % of the BDE. There are also extreme cases when this value exceeds the BDE value, and such an example is the fluorine molecule. This implies that in F_2, the covalent VB structure has antibonding character, which has been attributed to strong Pauli repulsion between bonding and lone electron pairs.[17,50,67–72] As a result, bonding in F_2, does not arise from spin-pairing stabilization, contrary to the widely held belief that such effects are characteristic of all homopolar chemical bonds. Instead, CSB provides an alternative bonding mechanism for systems where neither electrostatic interactions nor spin-pairing effects alone can adequately explain the bonding.

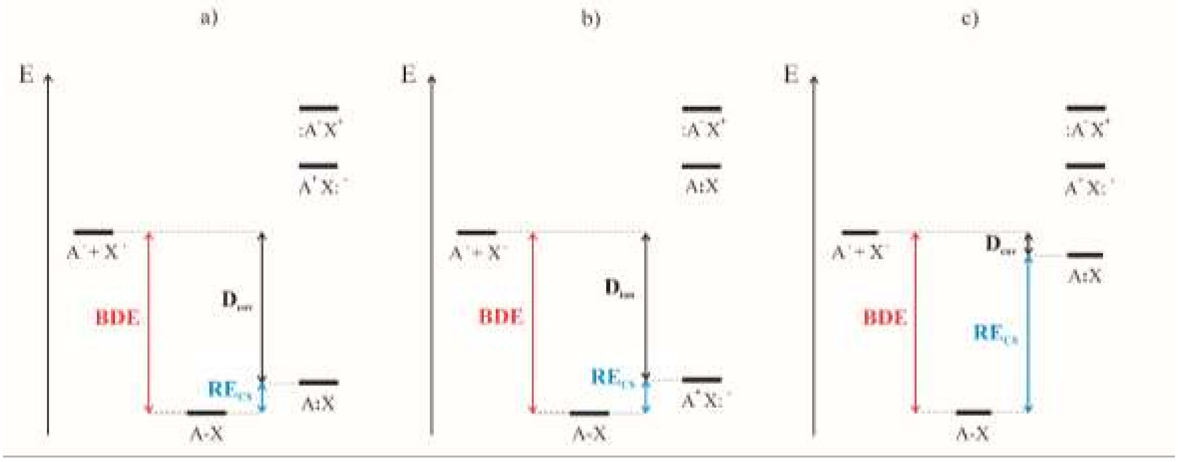

Fig. 2. VB interaction diagrams describing the classification of electron pair bonding: covalent (a), ionic (b), and charge-shift (c)

Studies have shown that the CSB family is broad and includes: homopolar bonds involving compact, electronegative, and/or lone-pair-rich elements; heteropolar bonds between such elements and others (e.g., metalloids like silicon and germanium); hyper-coordinated molecules; and bonds whose covalent components are weakened by exchange-repulsion strain.[20,50,53,73]

2.3. *Participants*

The research sample consisted of 47 chemistry students – 38 female and 9 male. This diverse group included students at different academic levels: 26 second-year undergraduate, 10 master's (MSc) students, and 11 doctoral (PhD) students. All participants were enrolled in chemistry courses essential for understanding chemical bonding, including General Chemistry, Physical Chemistry 1 and 2, and Molecular Modeling. Key terms related to chemical bonding (octet rule, atomic orbital, molecular orbital, etc.) and those specific to charge-shift bonding (e.g., resonance hybrid, bond dissociation energy, resonance energy) were covered during their university education.

Additionally, students attended a lecture prior to the practical exercise, during which all concepts related to CSB were explained. The study was conducted at the Faculty of Science, University of Kragujevac in Kragujevac, Serbia, and included internal students following the institution's curriculum.[74] The research was conducted in accordance with relevant laws and institutional guidelines and was ethically approved by Faculty's ethics committee (No. 180/XVIII-1). All three questionnaires were completed anonymously, and only students who consented to participate were included in the study. Participants were informed they could withdraw their consent at any time during the research.

2.4. *Instrument*

Three questionnaires (pre-, post-test, and survey) were administered to address the research questions and assess the potential impact of the practical approach. The test questions were reviewed by a team of chemistry education experts who were not involved in the implementation, ensuring the instrument's validity by evaluating its alignment with the targeted concepts and objectives. The reliability of the survey was assessed using Cronbach's Alpha coefficient, which yielded a value of $\alpha = 0.91$ – well above the recommended threshold of 0.70, indicating high internal consistency. Questions from both knowledge tests and the survey are provided in the Supplementary Material.

To evaluate potential changes in students' knowledge, five questions from the pre-test correlate to the first four questions on the post-test. The 4th and 5th questions from the pre-test were paired with the 4th question on the post-test, as they are conceptually related.

The survey was designed to examine students' attitudes and self-perceptions about their knowledge of chemical bonding, the usefulness of the practical approach they experienced, and views on ICT and the effectiveness of the practical class. Students were asked to respond to 20 items on a five-point Likert scale (1 – strongly disagree; 2 – disagree; 3 – neutral; 4 – agree; 5 – strongly agree) following the practical training. The distribution of responses to the final two post-test questions was intended to provide insight into students' understanding of the CSB concept. Additionally, responses to survey statements 7 – 12 were used to evaluate students' comprehension of the charge-shift bonding concept and to address the first research question.

2.5. *Practical training*

If students were asked to classify a series of molecules based on their type of chemical bonding, they would likely not distinguish between homonuclear diatomic molecules such as hydrogen (H_2) and fluorine (F_2). Most would probably categorize both as covalent, in line with the widely accepted Pauling bonding scheme illustrated in Figures 2a and 2b. It is important to note that in the 1930s, accurate VB calculations were not feasible. As a result, Pauling approximated that the resonance energy in homonuclear bonds – such as H–H and F–F, was zero. When full *ab initio* VB calculations later became available, this approximation was shown to be reasonably accurate for H_2, but not for F_2. In the case of F_2, the covalent VB structure involved in the resonance model was found to have an antibonding character (i.e., the energy of the covalent structure F: F is higher than that of two isolated fluorine atoms).[17,50,67–72] This striking difference in bonding mechanisms between H_2 and F_2 serves as a useful example for introducing the concept of CSB. Additionally, sodium chloride (NaCl) is included as a representative example of ionic bonding. For pedagogical purposes, the approach was designed around well-known molecules – H_2, F_2, and NaCl.

The practical class was based on ICT learning tools and incorporated various computational techniques to enhance students' understanding of chemical bonding. The goal of the practical training was to clarify abstract terms and concepts related to CSB, supplementing the lecture-based instruction. The CSB concept was introduced through calculations of the contributions of covalent and ionic VB structures, BDE, and RE_{CS}. The recommended duration of this unit was 90-minute session. Students were supervised by a teaching assistant throughout the exercise. Although students were already familiar with basic quantum chemical calculations from using the Gaussian program package, the input files required for the exercise were prepared in advance by the assistant. The XMVB (Xiamen Valence Bond)[75,76] input files were also prepared beforehand and explained at the beginning of the class. These files are available in the Supplementary Material, along with an .ods file containing all calculated energetic quantities of the studied bonds. Additional guidance on preparing XMVB input files can be found in a recent tutorial.[77]

The first task involved calculating the BDEs of the selected molecules, starting from experimentally determined bond lengths[78] (see Table 1). Two VB methods were used: VB Self-Consistent-Field (VBSCF) and Breathing Orbital VB (BOVB). These classical VB approaches and their methods are described in more detail elsewhere.[63,76] Each bond was modeled as a resonance between its covalent and ionic VB structures (Figures S1–S3). In VBSCF, a common set of orbitals is used for all VB structures, while in the BOVB wavefunction, different VB structures are represented using distinct sets of orbitals. VBSCF captures static correlation, whereas BOVB also includes dynamic correlation.

BDEs were calculated relative to the energies of the dissociation fragments using the preint utility provided within the XMVB software package. Reint input files are also provided in the Supplementary Material. All calculations were performed using the 6-31G basis set – a relatively small basis set chosen to ensure that students could complete the calculation within the allotted time frame. The resulting BDEs are summarized in Table 1. The BOVB method yielded significantly better BDE values than VBSCF, due to its superior treatment of electron correlation. However, the BOVB results are still different notably from the experimental values.[79]

It is important to note that more advanced BOVB-based methods can yield highly accurate BDE values, but these calculations are computationally more demanding and require a deeper understanding of VB theory.[80] At this point, students were introduced to the basics of electron correlation. As shown, F_2 is a strongly correlated system that requires high-level computational methods to accurately capture electron correlation effects. The discrepancy between the results in Table 1 and those from previous VB studies[80] is largely due to the modest basis set used. In the previous study,[80] more advanced BOVB calculations were employed, including a refined treatment of singly and doubly occupied active orbitals (the S-BOVB approach). This method accounts for an additional portion of dynamic electron correlation, but it is too complicated to present to students with limited experience in such a short timeframe.

Finally, it is worth emphasizing that all conclusions drawn about the bonding types in the molecules studied are fully consistent with those obtained from higher-level VB calculations.[80]

Table 2 presents the Chirgwin-Coulson weights of the VB structures for the examined molecules, calculated at the BOVB level of theory. The Chirgwin–Coulson weights are used to quantify the contribution of individual resonance structures (or valence bond structures) to the overall VB wavefunction.[56] The BOVB wavefunctions for H_2 and F_2 are dominated by the covalent VB structure, while for NaCl, the ionic structure (Na^+Cl^-) contributes most significantly. The remaining VB structures – ionic for H_2 and F_2, and covalent for NaCl, have small but non-negligible contributions.

These calculated weights clearly differentiate between ionic and covalent types, aligning with Pauling's bonding scheme (Fig. 2). However, the values do not indicate any distinction between the bonding in H_2 and F_2, despite their fundamentally different bonding mechanisms.

Table 1

Bond dissociation energy (BDE, in kJ mol^{-1}) at the VBSCF and BOVB levels, as well as experimentally determined bond dissociation energy (BDE, in kJ mol^{-1}) and bond lengths (r, in Å) for the studied molecules

Molecule	**BDE_{VBSCF}**	**BDE_{BOVB}**	**BDE_{exp}**	**r_{exp}**
H_2	393.2	393.2	435.8	0.741
F_2	0.2	76.4	158.7	1.412
NaCl	269.1	283.5	412.1	2.361

Table 2

Chirgwin-Coulson BOVB weights of VB structures given in %

Molecule	Weight of structures		
	Covalent structure	Ionic structures	
H_2	H : H	H^+H^-	H^-H^+
	79.4	10.3	10.3
F_2	F : F	F^+F^-	F^-F^+
	73.4	13.3	13.3
NaCl	Na : Cl	Na^+Cl^-	Na^-Cl^+
	23.5	76.5	0.0

The next task involved calculating the RE_{CS}. Resonance energy is defined as the difference between the energy of the most dominant VB structure in a given wavefunction and the energy of the wavefunction that includes resonance between the full set of VB structures. The energies of the single covalent structures for H_2 and F_2 and the ionic structure of NaCl were calculated first. Students then used these values to calculate D_{cov} for H_2 and F_2, and D_{ion} for NaCl. The D_{cov}/BDE and D_{ion}/BDE reveal the difference between the three bonding types.

In the case of H_2, D_{cov} equals 93.8 % of the total BDE, and for NaCl, D_{ion} represents about 88.4 % of the BDE – typical values for covalent and ionic bonds, respectively, within the VB theory framework. In contrast, for F_2, the D_{cov} is negative, indicating that the covalent structure – although dominant, has antibonding character. This behavior is attributed to the relatively short interatomic distance in F_2, which leads to strong Pauli repulsions between the bonding and lone electron pairs. This destabilizing repulsion outweighs the stabilizing effects of spin-pairing, a hallmark of CSB.

How to understand the stability and bonding in F_2?

The CSB offers an alternative bonding mechanism in F_2. Unlike covalent bonds, where stability arises from spin pairing, or ionic bonds, where electrostatic interactions dominate, CSB is primarily stabilized by the resonance energy resulting from covalent-ionic mixing. The RE_{CS} and $\%RE_{CS}$ values indicate that bonding in F_2 is not a standard covalent bond but rather CSB type. While RE_{CS} contributes only modestly to the BDE in H_2 and NaCl, in F_2, nearly all stabilization arises from resonance mixing of VB structures.

The data are summarized in Table 3. It is worth noting that the $\%RE_{CS}$ values obtained here differ numerically from those derived using more advanced VB methods. However, these differences do not affect the overall conclusions regarding the bonding types in the studied molecules.

Table 3

Energy stabilization of the covalent/ionic structure (D_{cov}/D_{ion}) and resonance energy (RE_{CS})values (kJ mol^{-1}) and percentage contribution of the resonance energy to the bonddissociation energy ($\%RE_{CS}$) in %

Molecule	D_{cov}/D_{ion}	RE_{CS}	$\%RE_{CS}$
H_2	368.8	24.4	6.2
F_2	–175.1	251.4	329.2
NaCl	250.7	32.8	11.6

3. RESULTS AND DISCUSSION

Given that the distribution of students' responses on the knowledge test and their evaluations of the practical approach did not follow a normal distribution, potential differences among the three groups were analyzed using the Kruskal-Wallis test, followed by Dunn's post-hoc test.

The data collected with the two knowledge tests are presented in Table 4. Based on the results, students provided a limited number of correct answers on the pre-test, particularly for questions related to resonance hybrid, resonance, and bond dissociation energy. This result suggests a lower-than-expected level of understanding, which may be attributed to inadequate teaching methods or instructional tools. Similar findings were reported in a previous study,[81] which highlighted students' limited mastery of chemical bonding theory and emphasized the need for improved teaching materials – especially for topics such as ionic and covalent bond formation, electron domain theory, and exceptions to the octet rule.

Table 4

Distribution of correct answers (%) on questions (Q) per pre- and post-test

		Pre-test					Post-test		
Q	**2nd year**	**MSc**	**PhD**	**Total**	**Q**	**2nd year**	**MSc**	**PhD**	**Total**
1.	96.15	100.00	100.00	97.87	**1.**	92.31	100.00	100.00	95.74
2.	92.31	100.00	100.00	95.74	**2.**	96.15	100.00	100.00	97.87
3.	10.64	0.00	0.00	10.64	**3.**	57.69	100.00	72.73	70.21
4.	34.62	40.00	81.82	46.81	**4.**	80.77	100.00	100.00	89.36
5.	46.15	60.00	54.55	51.06	**5.**	46.15	90.00	81.82	63.83
					6.	88.46	100.00	100.00	93.62

Most students' responses to the third question reflected a common but incorrect understanding. Only the CSB option and its corresponding representation were rated as accurate, yet 89.36% of students answered in terms of covalent bonding. Interestingly, none of the MSc and PhD students answered the question correctly. However, this did not hinder their overall performance, as they demonstrated strong understanding of other questions, particularly in the post-test. To the best of the authors' knowledge, most widely used textbooks still describe bonding in the F_2 molecule as covalent.

After the practical exercise – which aimed to make the concept of chemical bonding more accessible, there was a noticeable increase in the number of correct responses. The most significant improvement was observed in students' understanding of resonance and bond dissociation energy. The relatively unchanged distribution of correct answers to the first two questions suggests that students already had a solid grasp of the distinctions between covalent and ionic bonding, in contrast to findings from earlier studies.[24,82]

High scores on the final two post-test questions among MSc and PhD students indicate that the newly designed practical approach had a positive impact on their understanding. The large number of post-test correct responses to key questions (5 and 6) clearly shows that the practical training enhanced students' insight into chemical bonding theory and their comprehension of CSB. Their answers suggest that they understood the CSB concept and could identify molecules in which resonance energy is the dominant component of bonding energy. In contrast, undergraduate students struggled with questions 3 and 5, suggesting that the training may have been too advanced for their level.

Students' responses to the first two questions on both tests indicate a preference for familiar representations of covalent and ionic bonding. As shown in Figure 3a, most students used Lewis structures to represent bond formation and relied on simpler bonding models, consistent with findings from similar studies.[62] Only a small number of students answered using molecular orbital theory (Fig. 3b). On the other hand, some researchers[27,83,84] have reported misconceptions among students, such as the belief that ionic bonding involves electron sharing – an idea not supported by the findings of this study.

The authors also examined whether there were differences among student groups in their perceived knowledge of CSB. These differences were analyzed using appropriate statistical tests, and the results presented in Table 5.

As shown in Table 5, there was no significant difference among the groups in the number of correct responses to the sixth question ($\chi^2 = 3.456$, $p > 0.05$). However, significant differences were observed for the fifth ($\chi^2 = 7.856$, $p < 0.05$) and third questions ($\chi^2 = 6.092$, $p < 0.05$). Dunn's post-hoc test revealed significant pairwise differences for the fifth question between second-year undergraduate and MSc students ($p = 0.015 < 0.05$), as well as between second-year undergraduate and PhD students ($p = 0.041 < 0.05$). A significant difference was also found between second-year undergraduate and MSc students for the third question ($p = 0.014 < 0.05$).

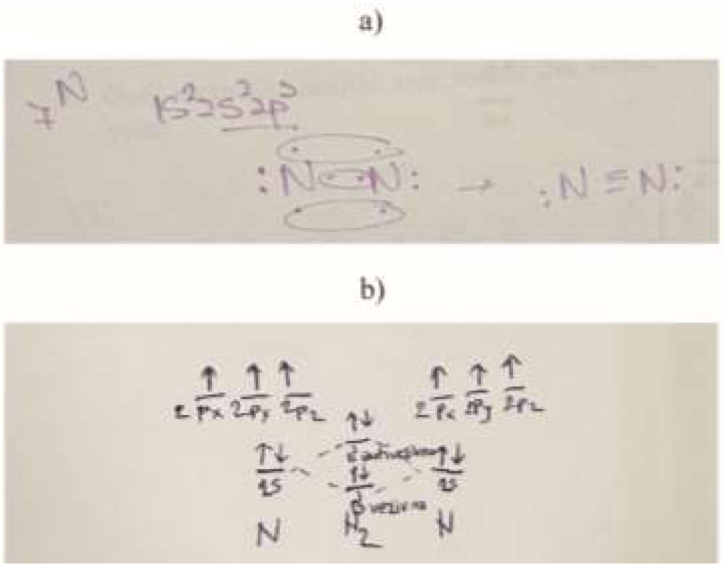

Fig. 3. Student's answer to the first question from the pre-test (a) and post-test (b)

Table 5

Descriptive statistics and Kruskal-Wallis test results of the effect of practical approach

	Level of study	%	df	χ^2	*p*-value	Significant difference
3rd Question	**2nd year**	57.69	2	6.092	**0.048**	2nd year – MSc
	MSc	100				
	PhD	72.73				
5th Question	**2nd year**	46.15	2	7.856	**0.020**	2nd year – MSc 2nd year – PhD
	MSc	90.00				
	PhD	81.82				
6th Question	**2nd year**	88.46	2	3.456	0.178	
	MSc	100.00				
	PhD	100.00				

Based on the results presented in Tables 4 and 5, second-year undergraduate students appeared to struggle with defining charge-shift bonding. However, they were still able to recognize examples from the CSB category, which may indicate functional knowledge. While it is important to introduce CSB theory at the undergraduate level, the practical training may be too demanding. Therefore, the authors recommend introducing CSB concepts theoretically through a few lectures at this level. It is important for students to be aware that new bonding models can more accurately explain the behavior of certain molecules.

Tables S14–S16 present descriptive statistics from the survey data. The first six statements focused on students' self-assessment of knowledge of chemical bonding theory. According to Table S14, most students considered their knowledge of chemical bonding to be acceptable. Students generally felt confident in their understanding of individual concepts like ionic and covalent bonding. Interestingly, PhD students rated their knowledge the lowest (mean = 2.45), which may reflect a tendency to be more self-critical and aware of their knowledge limitations. These findings align with the growing emphasis on strengths-based professional development in many graduate programs.[85]

Mean values of students' responses to statements 7–12 (Table S15) indicate an overall positive perception of the practical approach. Item 12 was examined specifically to identify potential differences between groups of students, but Kruskal-Wallis test showed no significant difference (χ^2 = 1.331, $p > 0.05$).

All mean values in Table S16 related to ICT and the efficiency of the practical class are satisfactory, except for item 19. These results suggest a need to further develop ICT competencies among students – skills that are increasingly recognized as essential worldwide.[44,47] The findings also support the idea that ICT positively influences student engagement and motivation.[42,43,47,86,87,88] Item 13 was investigated peculiarly, to reveal potential differences between groups of students, but Kruskal-Wallis test again showed no significant difference ($\chi^2 = 5.506$, $p > 0.05$). Based on these results, students across all groups perceived the practical approach as manageable and not overly demanding.

Table 6

Kruskal-Wallis test results of the comparison of the students' attitudes

Items	**Level of study**	**df**	χ^2	*p*-value	**Significant difference**
1–6	**2nd year** **MSc** **PhD**	2	0.035	0.983	
7–12	**2nd year** **MSc** **PhD**	2	7.716	**0.021**	2nd year – PhD MSc – PhD
13–20	**2nd year** **MSc** **PhD**	2	0.245	0.885	

According to the Kruskal-Wallis test results presented in Table 6, there were no significant difference among the groups in their attitudes regarding their knowledge of chemical bonding, or their views on ICT and the efficiency of the practical class. However, a significant difference was found in students' perceptions of the usefulness of the practical approach they experienced ($\chi^2 = 7.716$, $p < 0.05$). Dunn's post-hoc test revealed significant differences between second-year undergraduate and PhD students ($p = 0.031 < 0.05$), as well as between MSc and PhD students ($p = 0.009 < 0.05$).

PhD students found the practical approach more efficient. This finding is expected, as PhD students often demonstrate greater curiosity, a stronger desire to learn new concepts, and a higher level of motivation for professional development.[89,90] Students' responses to the second group of survey questions also suggest that the practical training may be more suitable for MSc and PhD students than for undergraduates.

4. CONCLUSIONS

Chemical bonding is one of the foundational concepts in chemistry that students encounter throughout their university education. To fully understand this concept, students must be familiar with various mathematical and physical principles, as chemical bonds cannot be directly observed in a laboratory setting. Because bonding is both complex and abstract, it is prone to misconceptions, making it essential to approach the topic from multiple perspectives.

This paper aims to offer a fresh perspective and deeper insight into this fundamental area of chemistry. At the same time, it emphasizes the importance of keeping the material accessible and predictive for students. Accordingly, the authors designed and implemented a practical approach to teaching chemical bonding. The paper presents unique instructional materials that combine modern teaching tools with classical valence bond (VB) theory.

The primary goal of the practical training was to introduce chemistry students to the concept of charge-shift bonding using contemporary teaching methods. While the authors acknowledge the limitations of the sample size and refrain from generalizing the findings, the results nonetheless offer valuable insights into effective teaching practices. The proposed approach not only simplifies the learning of complex bonding theories but also enhances student engagement, paving the way for a deeper and more meaningful understanding of chemical bonding.

Based on the data collected, the authors believe that MSc and PhD students are well-positioned to comprehend new bonding concepts through the proposed practical class. At the upper undergraduate level, it is important to expose students to emerging scientific ideas, such as CSB, to keep them aligned with current developments in the field. While practical training may be too demanding for undergraduate students, they should still be introduced to CSB and similar advanced concepts through theoretical lectures in order to build foundational knowledge.

Participation in the practical class led to an overall positive response from students regarding the usefulness of the practical approach and their perceived knowledge gains. This study demonstrates that innovative, hands-on teaching strategies can significantly improve students' understanding of chemical bonding, particularly at the postgraduate level. However, careful attention must be paid to the design and implementation of such activities to ensure they are appropriately challenging for each academic level. These findings support a more differentiated and inclusive approach to teaching advanced bonding concepts, ultimately fostering a deeper comprehension and appreciation of chemistry among students.

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