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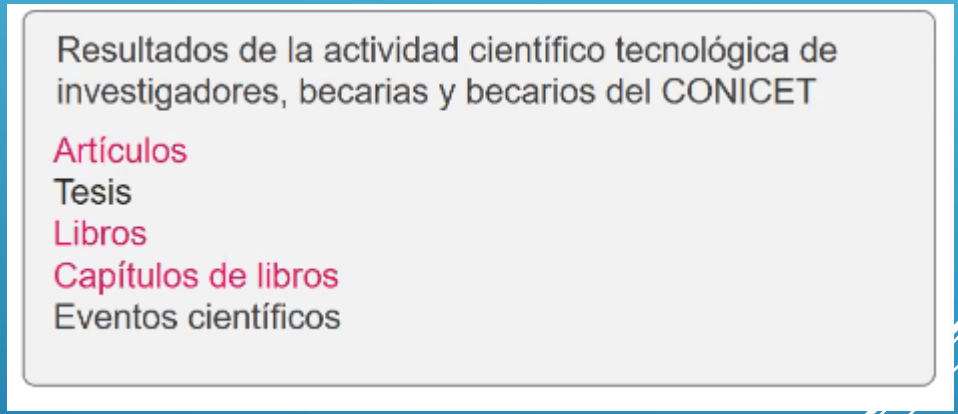

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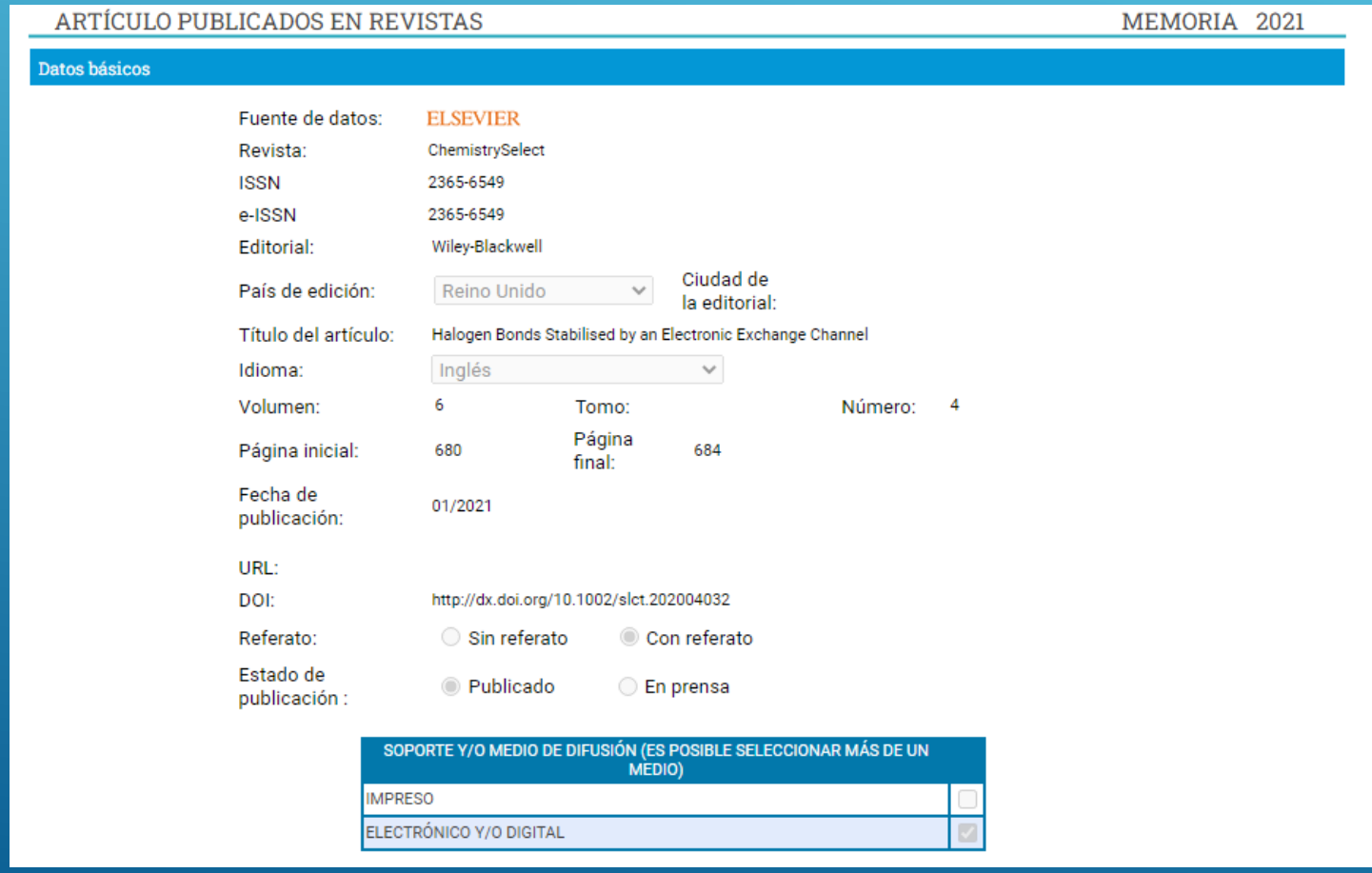

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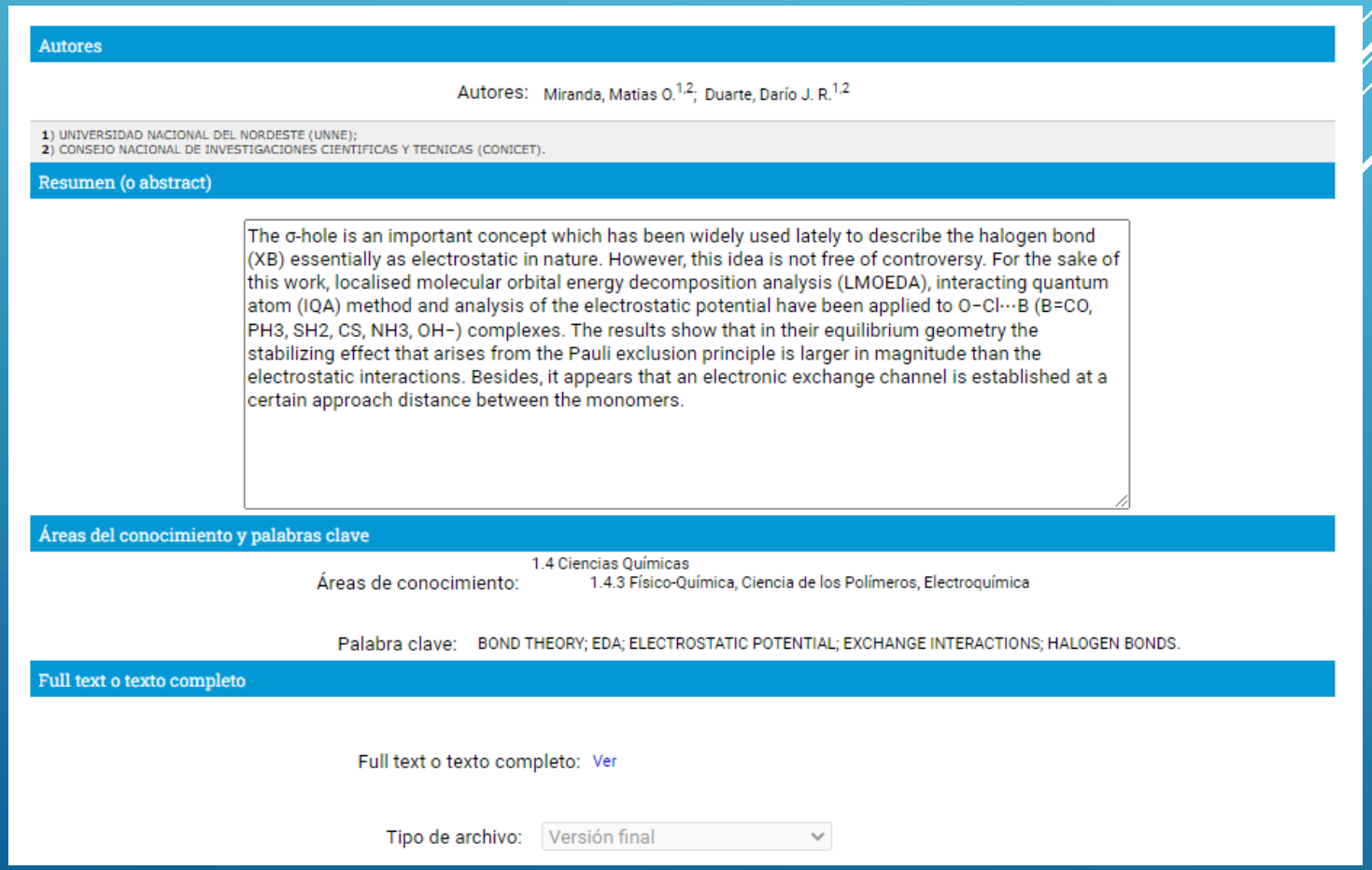

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Resumen (o abstract)

The σ-hole is an important concept which has been widely used lately to describe the halogen bond (XB) essentially as electrostatic in nature. However, this idea is not free of controversy. For the sake of this work, localised molecular orbital energy decomposition analysis (LMOEDA), interacting quantum atom (IQA) method and analysis of the electrostatic potential have been applied to O−Cl···B (B=CO, PH3, SH2, CS, NH3, OH−) complexes. The results show that in their equilibrium geometry the stabilizing effect that arises from the Pauli exclusion principle is larger in magnitude than the electrostatic interactions. Besides, it appears that an electronic exchange channel is established at a certain approach distance between the monomers.

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Halogen Bonds Stabilised by an Electronic Exchange Channel

Matias O. Miranda[a, b] and Darío J. R. Duarte*[a, b]

Dedicated to Professor Nélida M. Peruchena

The σ-hole is an important concept which has been widely used lately to describe the halogen bond (XB) essentially as electrostatic in nature. However, this idea is not free of controversy. For the sake of this work, localised molecular orbital energy decomposition analysis (LMOEDA), interacting quantum atom (IQA) method and analysis of the electrostatic potential have been applied to O–Cl···B (B = CO, PH_3, SH_2, CS, NH_3, OH^-) complexes. The results show that in their equilibrium geometry the stabilizing effect that arises from the Pauli exclusion principle is larger in magnitude than the electrostatic interactions. Besides, it appears that an electronic exchange channel is established at a certain approach distance between the monomers.

It is well known that halogenated oxides (OI, OBr, OCl and at a lesser extent the OF) play an important role in the chemistry and oxidising capacity of the troposphere.[1] The interacting halogen bonding that these oxides can form have peculiar characteristics. Zhu et al. have studied the solvation of a BrO radical using adaptive buffered force quantum mechanics/molecular mechanics (QM/MM) dynamics simulations. Their results show that "…the BrO radical prefers to be solvated at the surface of the water slab, rather than the interior region of the water slab despite its high affinity to water".[2] Besides, two types of OBr-OH_2 contacts were observed (see figure 4a, complex3 and complex9 of reference 2), complex3 seems to be a classic halogen bonds (XBs), while in complex9 the Br atom interacts with two O atoms. Gálvez and Gómez have studied the hydrates of chlorine monoxide [ClO-$(H_2O)_n$, n = 1-6] by means of DFT (B3LYP) and ab initio [MP2 and CCSD(T)] methods with large sets of base functions. They have found two different intermolecular interactions, conventional hydrogen bonds and OCl-OH_2 contacts. Some of these latter interactions have the typical geometric characteristics of XBs, while others present considerable deviations compared from the conventional XBs of 180 degrees.[3]

The σ-hole is an important concept which has been widely used lately to describe non-covalent interactions between a covalently-bonded atom of groups IV–VII in the periodic table and a Lewis base.[4,5] This concept was first used by Politzer et al. for describe to XBs. Then, Clark, Murray and Politzer showed that known features of XBs can be understood through the electrostatics/polarization plus dispersion interpretation.[6–8]

There is a large number of studies based on the σ-hole concept that allowed the IUPAC to establish that XBs are primarily electrostatic in nature.[9] However, Stone showed that the geometries of the XBs are not always determined by the electrostatic component.[10] Syzgantseva et al revealed that the exchange component is very important for the stabilisation of these complexes in their equilibrium geometries.[11] Bartashevich et al and Bora et al found that bifurcated XBs presents a strong covalent character.[12,13] Moreover, we have recently shown that some XBs are quantum in nature. In this same work, we have also shown that the σ-hole magnitude can be interpreted as a channel that facilitates the electronic exchange between interacting atoms.[14]

On the other hand, from the works of Tsirelson et al,[15] Gadre et al[16] and Salahub et al[17] the topology of the electrostatic potential [$\phi(\mathbf{r})$] has shown to be a reliable tool, especially to understand the role of electrostatic in molecular interactions.[18–21] For example, the stability of anion-anion interactions bound by hydrogen bonds (HBs) in gas phase has been explained by attractive forces localized in a volume situated in the intermolecular region of the HB and defined as the electrostatic attraction region (EAR). This region was determined by the topological analyses of the electron density and of the $\phi(\mathbf{r})$, and by the electric field lines (EFL).[18] A nucleophilic region of a Lewis base on a surface of the molecule can be revealed as a minimum with negative value, on the topology of $\phi(\mathbf{r})$.[19] Besides, the $\phi(\mathbf{r})$ has been shown, for non-covalent interactions, to have positive values between two interacting atoms.[14,22] So, it is interesting to see how the topology of $\phi(\mathbf{r})$ function varies during the formation of XBs as well as their relationship with some energy decomposition analysis (EDA) components. For this purpose, we have studied the selected complexes among the halogenated oxide OCl and the Lewis bases CO, PH_3, SH_2, CS, NH_3 and OH^-.

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(charge transfer, electron density polarization, etc.) occurs within a system, Coulombic terms necessarily appear".[19b]

In conclusion, we have reported the relationship between some parameters of $\phi(\mathbf{r})$ and the quantum and classical effects obtained with LMOEDA and IQA schemes. At the geometry of equilibrium, the stabilizing effect that arises from the Pauli exclusion principle is larger in magnitude than the electrostatic interactions. Coulombic forces are important at long range and they are in according with σ-hole concept. The variations of V_{cp} over the LP of the Lewis base in conjunction with the variations of E_{el} and E_{ex} terms of LMOEDA scheme with the intermolecular distance seem to indicate that an electronic exchange channel is established at a certain approach distance between the monomers. Finally, the topology of $\phi(\mathbf{r})$ is a reliable tool to detect well-defined lone pairs and to understand in depth the electronic changes that occur in the process of formation of XBs.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords: Halogen bonds · Exchange interactions · Electrostatic potential · EDA · Bond theory

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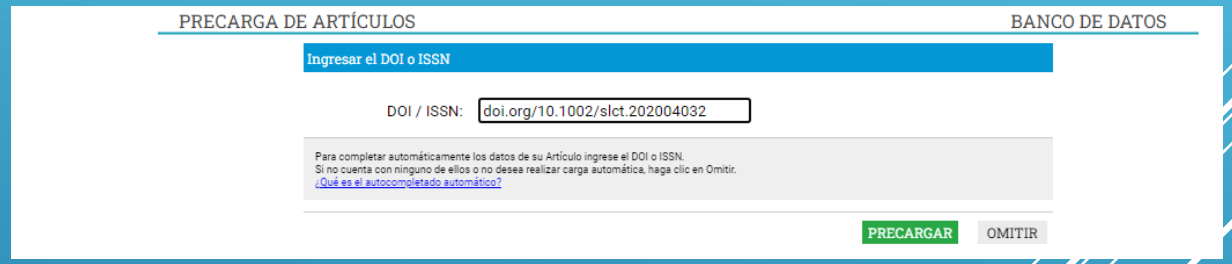

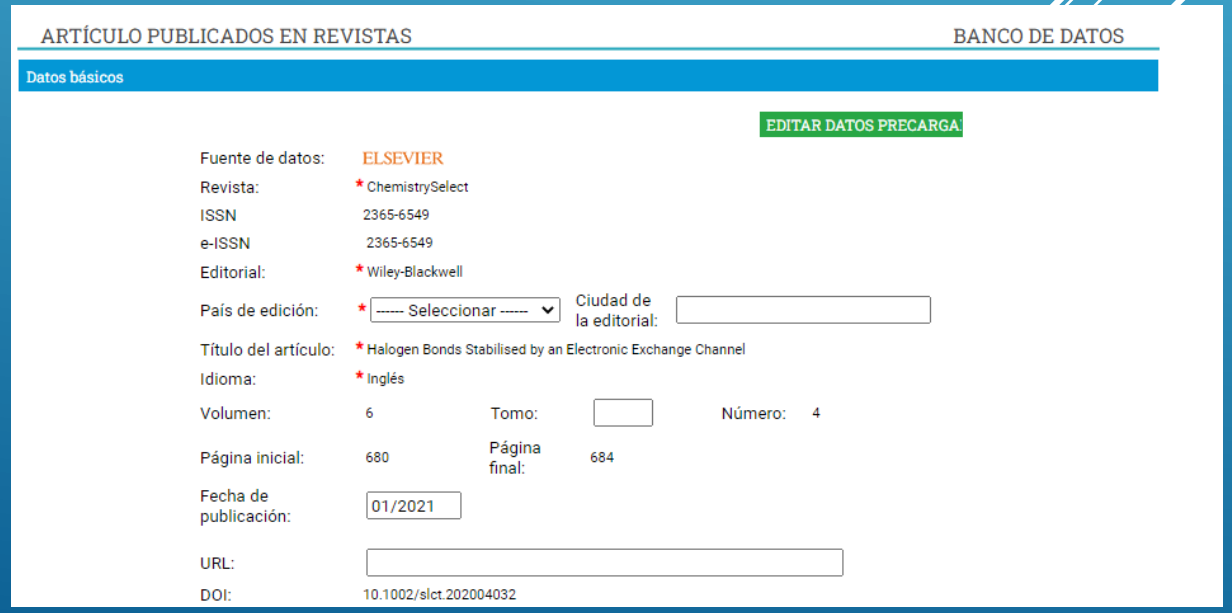

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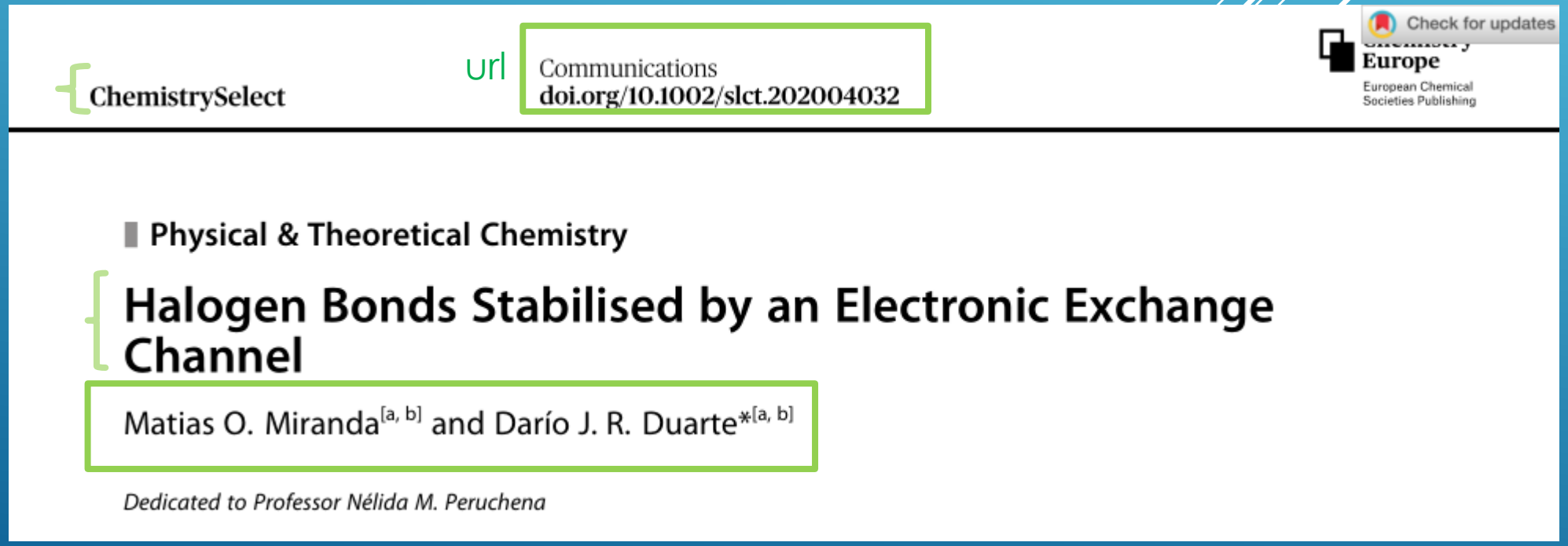

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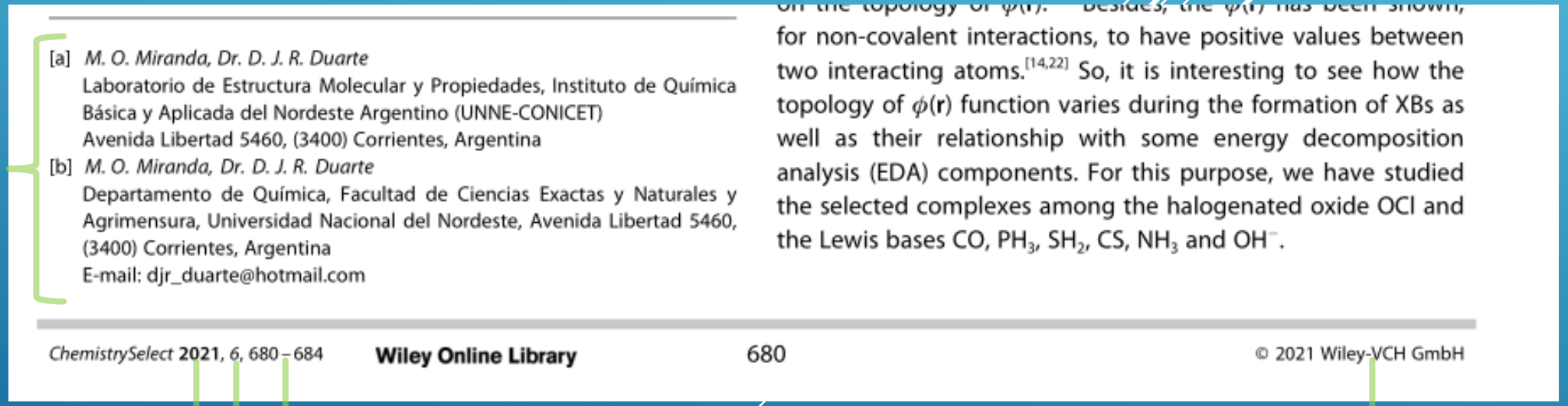

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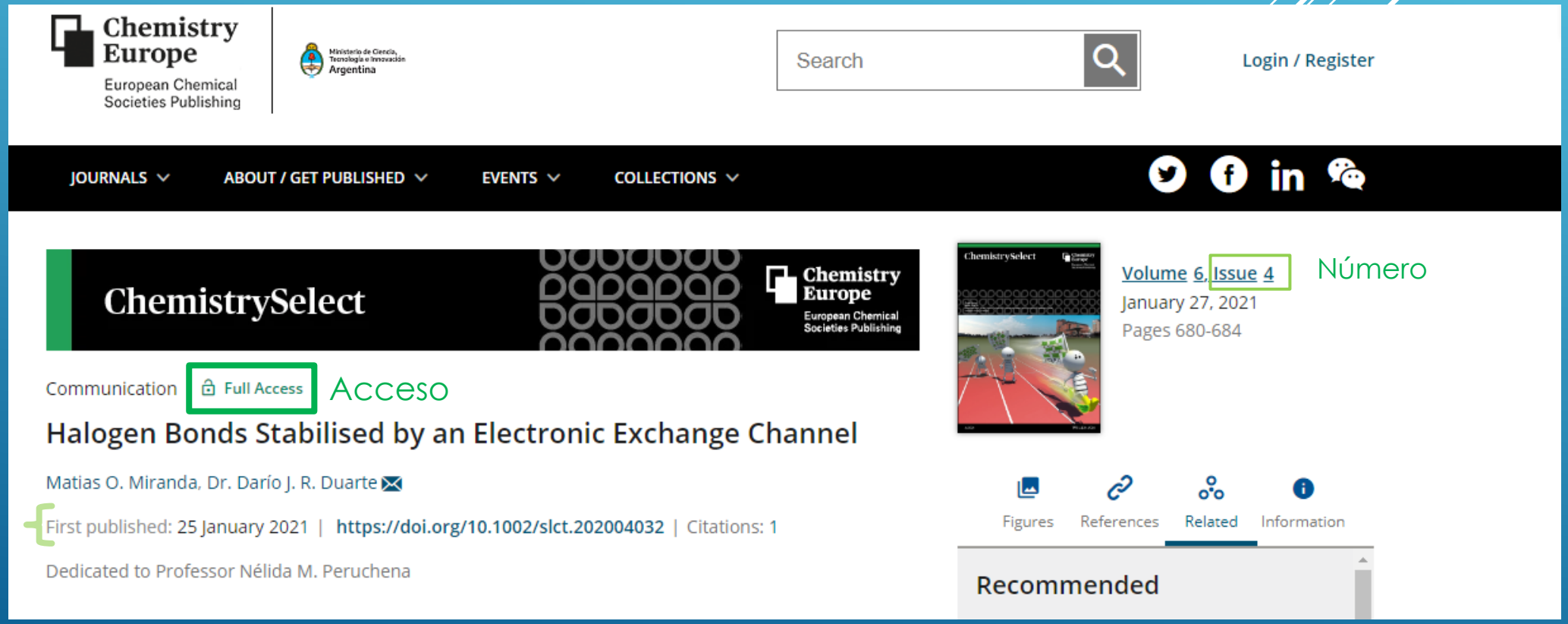

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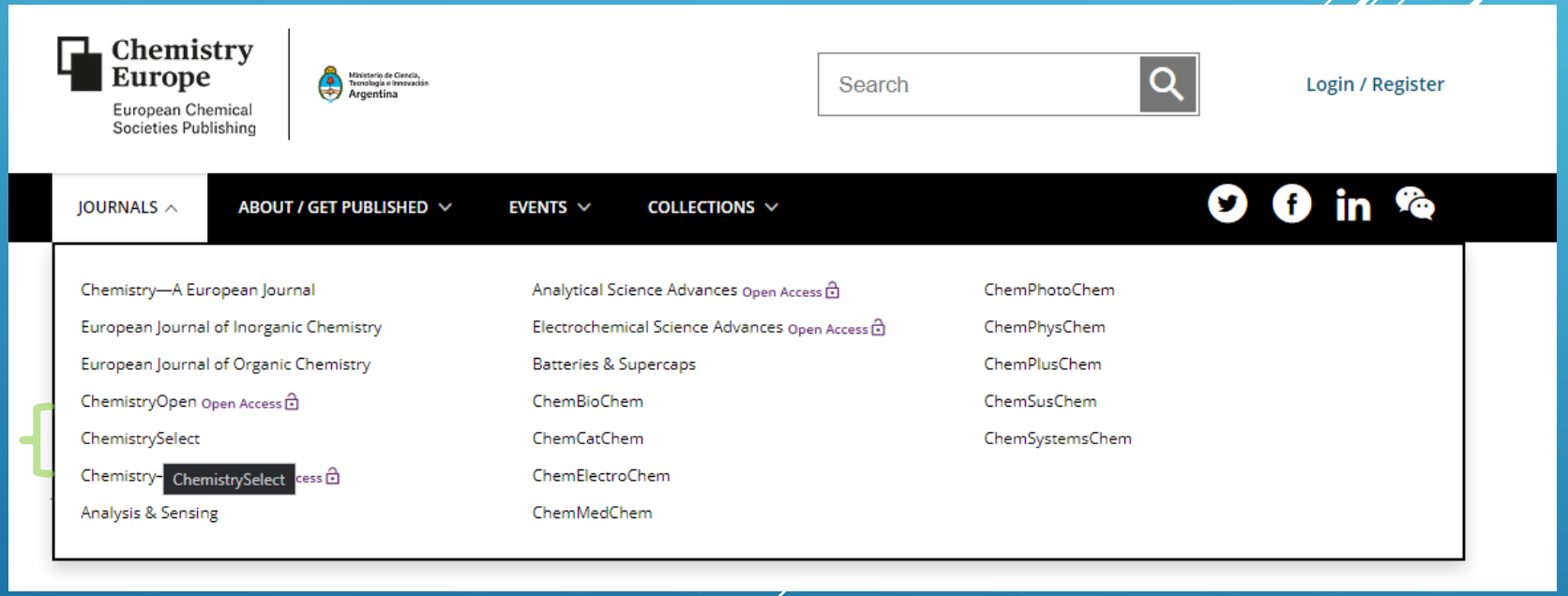

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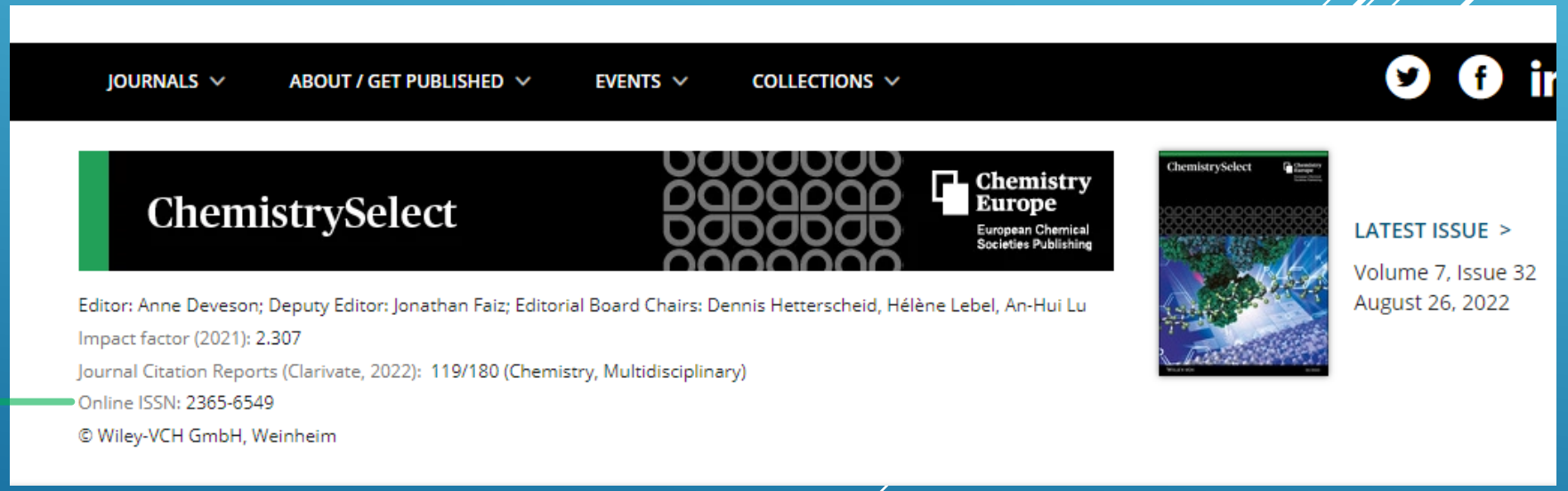

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