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ARTICLE *in* JOURNAL OF CHEMICAL EDUCATION · JULY 2014

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A Simple Demonstration of Atomic and Molecular Orbitals Using Circular Magnets

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ABSTRACT: A quite simple and inexpensive technique is described here to represent the approximate shapes of atomic orbitals and the molecular orbitals formed by them following the principles of the linear combination of atomic orbitals (LCAO) method. Molecular orbitals of a few simple molecules can also be pictorially represented. Instructors can employ the method to demonstrate the application of the LCAO method, which can help students better understand the bonding principle.

KEYWORDS: *High School/Introductory Chemistry, Demonstrations, Hands-On Learning/Manipulatives, MO Theory*

INTRODUCTION

In an introductory chemistry course, a student must encounter the concept of orbitals and formation of chemical bonds through the LCAO approach. Pictorial presentations of different types of atomic orbitals and the molecular orbitals resulting from their linear combinations are an essential tool for the understanding of the bonding principle. Although a number of standard textbooks, animated video files, and software packages are available for this purpose, nevertheless, better understanding of this topic can be achieved through live classroom demonstrations of the phenomenon by the help of simple means, like iron filings and magnets. Magnets previously have found plenty of utilization by educators in describing different elementary chemical concepts, like VSEPR theory,[1] visualization of biomolecules,[2] solubility,[3] orbital filling,[4] crystal lattice and hydrogen bonding,[5] paramagnetism,[6] oil spill adsorption,[7] nucleophilic substitution mechanism,[8] redox reactions,[9] etc.

Interestingly, L. F. Druding[10] also used bar magnets and iron filings to demonstrate sigma and pi bonding formation. Well-dried iron filings, placed in a region of magnetic field, serve the purpose of mapping the magnetic field density, which could be regarded as the representation of electron density in molecules.[1a,10]

Motivated by the pioneering work of L. F. Druding[10] where two bar magnets were used to represent the bonding/antibonding interactions, we tried to modify and extend the work. In Druding's work two bar magnets were arranged in end-on and side-on fashion along the imaginary bonding axis to depict the sigma and pi bonding/antibonding interaction, respectively. However, this brilliant and innovative procedure faces shortcomings in some cases, like presentation of p-orbital nodes, qualitative visualization of individual atomic orbitals, and their different way of linear combinations and bonds in bent molecules. We have modified the technique by using ring/cylindrical magnets, which can easily represent each lobe of an orbital, and with proper arrangements of these magnets, molecular orbitals with nodes can also be visualized. Overall, following this present work, educators may show live formation of molecular orbitals from atomic orbitals in a convenient way.

However, here it is important to note that interactions between two magnetic poles and between two orbital lobes are very much dissimilar in nature. Whereas, according to the LCAO principle, orbital lobes with similar sign (+,+/−,−) interact to form bonding orbitals and orbital lobes with opposite sign (+,−) interact to form antibonding orbitals, in the case of magnets, opposite poles (north and south) attract each other and similar poles (north−north/south−south) repel each other. Thus, to avoid the confusion and serious misconception among the students, it is advisible that the instructor should clearly discuss all the theoretical principles behind the orbital and magnetic interactions.

METHOD

All the ring and cylindrical magnets were collected from damaged audio speakers (Figure 1). These magnets have been used because these are easily available and of low price. North and south poles of the magnets can be determined using a compass (Figure 2). **CAUTION!** Protective goggles and gloves are recommended during the demonstration to avoid direct contact with the iron filings. Keep electronic devices and metal objects away from the magnets.

A smooth wooden board was fitted about a few centimeters above the ground. A thin white paper was placed on this

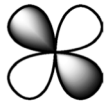
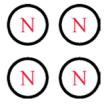
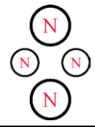
Published: July 22, 2014

dx.doi.org/10.1021/ed400803u | *J. Chem. Educ.* 2014, 91, 1505−1507

Figure 1. Audio speaker ring magnets.

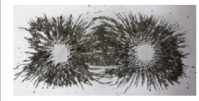
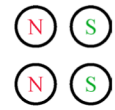
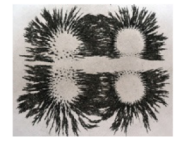
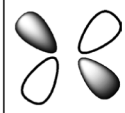
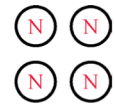
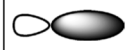
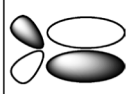
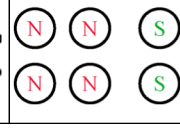
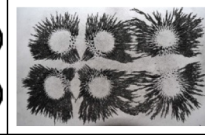
Figure 2. Determination of poles of a ring magnet with a compass.

Table 1. Representation of Some Atomic Orbitals

Atomic Orbitals	Approximate Pictorial Representation	Arrangement of Magnets That Have Poles Upwards	Illustrative Description of Orbital by the Map Created by Iron Filings
s			
p			
d_{xy}, d_{xz}, d_{yz}, $d_{x^2-y^2}$			
d_{z^2}			

wooden board and was fixed with four board clips. A small amount of iron filings was uniformly sprinkled on the paper. To represent a bonding or an antibonding interaction, two opposite poles (north and south poles) or two similar poles (either two north poles or two south poles) were placed side by side. The demonstration was set up by placing the ring and/or cylindrical magnets below the flat wooden platform on which the iron filings were carefully placed. When the wooden board is gently tapped by a hammer, the iron filings will arrange themselves in a pattern according to the mutual interaction between the magnets to form the shape of the desired AO or MO. Nodes in p and d AOs and different MOs can also be made prominent when magnets are placed at suitable distances. However, as enough closeness of a pair of magnets may result in sticking together due to attraction or pushing away due to

Table 2. Representation of Some LCAO

LCAO Descriptions	Approximate Pictorial Representation	Arrangement of Magnets That Have Poles Upwards	Illustrative Description of MO by the Map Created by Iron Filings
s + s			
s − s			
p + p			
p − p			
p + s			
d + p			

repulsion, it is better to use either a thin wooden separator between them or adhesive tape to hold them in desired positions.

Following this method, both AOs and MOs can be easily represented. For example, in Table 1, pure s, p, and d AOs are shown, and in Table 2, a few MOs formed from the interaction of two such pure AOs are presented. With an adequate number of magnets, MOs formed from more than two AOs can also be shown (figure not shown).

DISCUSSION

This method is also helpful to represent the molecular orbital description of small bent molecules like $CH_2{=}CH{-}CH_2^+$ ion (conjugated π system) as is shown in Figure 3. Students under the supervision of their instructor may also try the method for other molecules especially which have their representative orbitals lying on the same plane (i.e., the plane of the paper). MOs, for instance, resulting from δ-bonding cannot be shown by this method because the participating $d_{xy}/d_{x^2-y^2}$ orbitals do not lie in same plane. Moreover, magnets of different sizes can also be introduced to represent the MOs formed by dissimilar sized atomic orbitals.

However, despite the usefulness of this method, one may not be able to present some typical cases, like lateral interactions between s and p orbitals and different atomic orbitals resulting from hybridization schemes.

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dx.doi.org/10.1021/ed400803u | J. Chem. Educ. 2014, 91, 1505−1507

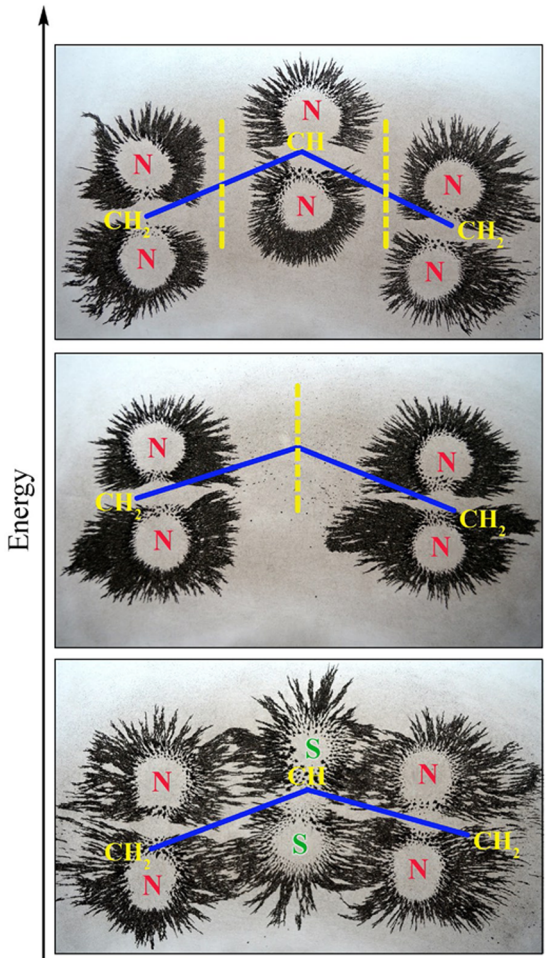

Figure 3. Energy level diagram of π MOs of $CH_2{=}CH{-}CH_2^+$ ion.

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

Thanks to the Blue Earth Workshop (Jadavpur University, Kolkata) for supplying cast iron filings free of cost. Thanks also to Monojit Mitra for his valuable contributions. The award of Senior Research Fellowships to M.C. and R.S.D. by the Council of Scientific and Industrial Research (New Delhi, India) is gratefully acknowledged.

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