Contents list available http://www.kinnaird.edu.pk/

Journal of Natural and Applied Sciences Pakistan

Journal homepage: http://jnasp.kinnaird.edu.pk/

QUANTUM MECHANICAL EXPLORATION OF HOMO- AND HETERO-DIATOMIC MOLECULES USING THE LINEAR COMBINATION OF ATOMIC ORBITALS APPROACH

Abdulwahhab Alkuwafi[1*]
[1]Department of physics, Faculty of Science, Omar Al-Mukhtar University, Albidah, Libya

Article Info

*Corresponding Author
Email: abdelwahab.alkuwafi@omu.edy.ly

Abstract

This research endeavors to model and examine the quantum mechanical behavior of Homo- and Hetero-Diatomic Systems utilizing the Linear Combination of Atomic Orbitals (LCAO) approach, directing attention to wave function localization and energy distribution. Simulations were carried out on two-dimensional atomic clusters by means of the LCAO Workbench, assessing bonding and antibonding states for both symmetric (Homo-Diatomic) and asymmetric (Hetero-Diatomic) Molecules. The systems were distinguished by altering atomic radii and potential depths. The Homo-Diatomic Molecules displayed symmetric bonding and antibonding states by reason of identical atomic properties, yielding closely spaced energy levels. By comparison, the Hetero-Diatomic Molecule demonstrated pronounced asymmetry, with the atom of high radius dominating wavefunction localization. Bonding states indicated notable wavefunction overlap and lower energy, whereas antibonding states revealed minimal overlap and higher energy. These findings highlight the impact of atomic asymmetry on molecular stability and electronic structure. The investigation showcases the versatility of the LCAO approach in modeling complex atomic interactions, delivering a sturdy framework for future nanoscale quantum examinations.

Keywords

Linear Combination of Atomic Orbitals (LCAO), Wavefunction Localization, Molecular Stability, Diatomic Systems

1. Introduction

One of the remarkable concept that one may encounter while studding the material and solid state physics is when two or more atoms are combined together. In the event that many atoms are brought close, their associated wavefunctions start of overlap notably, the energies, and all the qualitative traits of the overlapped wavefunctions, experience alterations. The Linear Combination of Atomic Orbitals (LCAO) approach continues to be an essential tool in solid-state physics and quantum chemistry, underpinning in the realm of atomic and molecular electronic structure computations. Through the depiction of electron wavefunction as an aggregate of –atomic orbital contributions centered on each atom enclosed within a system, LCAO clarifies the complex challenge in the assessment of the electronic structure of solids (Evarestov, 2012). In the domain of solid-state physics, the LCAO method demonstrates significant worth for investigating the electronic properties of materials. It provides researchers equipped to interpret and predict atomic interactions within a solid, which are essential to the exhibition of physical characteristics for instance; magnetism, conductivity, and optical properties (Cardona, 2007). The base line principle of LCAO argues that the electron wavefunction in a solid is an aggregate of wavefunctions of isolated atoms, taking into consideration their interdependent relationships. The multifaceted nature of the LCAO approach is applicable in numerous systems, such as periodic solid crystals, where it exploits the periodic potential to break down systematically the electronic structure covering a wide array of materials extending from pure metals to semiconductors and insulators (Slater, 1954). The central purpose of this research is to conduct simulations of two-dimensional atomic clusters utilizing LCAO approach executed via a Pascal-based programming environment. This simulation project incorporates within Consortium for Upper-Level Physics Software (CUPS). The LCAO Workbench is an elegant computational framework created to assist a dynamic analysis of the LCAO approach under the scope of solid-state physics. This software supplies a straightforward interface via which users can alter and visualize the properties of simple 2D atoms, each depicting a state of single electron. By modifying the basic parameters of these entities, such as coordinates in x-y plane, diameter, and quantum numbers, users can examine the emergent quantum mechanical behavior of the studied system. The LCAO Workbench thus operates as vital academic and research tool, providing a hands-on approach for insight the core concepts controlling electron behavior in solid clusters, and its consequences for electronic properties and material science (Silsbee, 1997).

1.1 Two Dimensional Atomic Clusters

A hydrogen-like atoms are quite simple. They are characterized by their piecewise constant potential that affords them a remarkably straightforward wavefunction. The bound state for every atom, there are Bessel functions of the first type in the interior of the atom ($r < R$), and another customized Bessel functions of the second kind, in

the exterior ($r > R$)[1] (Wang, 2024). The boundary conditions that influence the atomic wavefunctions, are that the value and derivative of the wavefunction must be properly rescaled (normalization of the wavefunction). The well-known time-independent Schrödinger is

$$\frac{-\hbar^2}{2m}\nabla^2\psi(r,\theta) + V(r,\theta)\psi(r,\theta) = E\psi(r,\theta) \quad \ldots(1)$$

In this study we are concerned with the ground state of atoms with single electron and cylindrically symmetric potential ($V(r,\theta)$ is actually a function of r only). This condition reduces the Schrödinger equation in cylindrical coordinate system to

$$\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi(r)}{\partial r}\right) + V(r)\psi(r) = E\psi(r) \quad \ldots(2)$$

In fact, Equation (2) is an eigenvalue equation with the eigenvalues considering the energies of the quantum states, and the associated eigenfuntions considering the atomic wavefunctions that we are interested in. In this context, the eigenvalue problem can be expressed as

$$H_{ato.}\psi = E_{ato.}\psi \quad \ldots(3)$$

where the left hand side of the above expression is obviously ($H_{ato.}\psi$) the atomic Hamiltonian. In this problem, the piecewise constant $V(r)$ or the potential constant takes different values at different situations in space. Specifically, conceptualizing the atom as a cylindrical model (square well potential problem) with its radius and depth being changing will make the solution of Equation (2) pretty simple. Actually, they are the Bessel function $J_{Bessel}(0,x)$ and the modified function $K_{Bessel}(0,x)$[2]. For the purpose of achieving the complete wavefunction for a specific atom, two boundary conditions are required to be met, and the wavefunction necessary to be adequately normalized. Conventional boundary conditions are employed: $\psi(r)$ has to be continuous at the discontinuity in the potential; $\partial\psi(r)/\partial r$ needs to maintain continuity at the point of discontinuity.

1.2 Interaction of Atomic Wavefunctions

Upon atom assembly to form an atomic cluster, their associated wavefunctions are no longer in isolation. Alternatively, they interact and influence the surrounding atoms and their associated wavefunctions as well. This communication between atoms is commonly known as 'cluster states' that represents the new formed ground states of the integrated system. Surprisingly, the new cluster states are significantly different from the isolated states. The interplay between atomic wavefunctions is vital in evaluating the electronic structure of the formed cluster. The wavefunctions overlap, giving rise to two crucial states; bonding and antibonding states that govern the stability and properties of the solid state matter. This occurrence carries special importance in nanoscale systems, at points where quantum influences are notable, and the electronic properties are substantially influenced by these wavefunction interactions (Pal, 2021) and (Kanada-En'yo, 2021).

1.3 LCAO Theory

As mentioned above, in the event that atoms come together, their wavefunctions reflect the effect of the

[1] In this context r is the distance measured from the center of the nucleus and *R* being the diameter of the atom.

[2] $J_{Bessel}(0,x)$ is characterized by Bessel differential equation of order zero and is exhibits regularity at the origin. On the other hand, $K_{Bessel}(0,x)$ exhibits global regularity With the exception of a simple pole at the origin.

interaction in the formed system. There will be cluster states that are consistent with eigenstates of the integrated atomic potentials. In particular, solving for the exact eigenstates of this system demands considerable computational power. Since we are endeavoring for a "real time" system that allows the researcher to facilitate interactive modifications to the shape and position of atoms in the cluster, an exact solution lies beyond the computational power of standard desktop machines. On the other hand, there is a prominent approximation that leads to qualitatively correct and reasonably close quantitative outcomes. This approach is LCAO. The principle is that the interaction potential between atomic neighbors operates as disturbance, efficiently combining the atomic states into an overall molecular or cluster state. Consequently, one may use the atomic stats as a proficient collection of primitive states for establishing the combined states of the cluster of atoms (Cramer, 2013). In this simulation, we will deal only with atomic ground states for the sake of simplicity, let the ground state of the ith atom be ψ_i. The new configuration cluster state can be expressed as

$$\Psi = \sum_{i=1}^{N} c_i \psi_i \qquad \ldots(4)$$

in the cluster state Ψ, the c_i's are the probability amplitudes for each individual atomic state. The c_i's values can merely evaluated with the aid of the associated eigenvalue problem:

$$H_{Total}\Psi = E\Psi \qquad \ldots(5)$$

the total Hamiltonian (H_{Total}) takes into consideration the interatomic and atomic interactions such that; $H_{Total} = H_{Atomic} + H_{Interatomic}$. The atomic part of the Hamiltonian takes into account each individual term in the cluster wavefunction. Utilizing Equation (5) we can easily end up with the atomic energies. Writing each atomic state as $|i>$, then the eigenvalue equation (Equation (5)) becomes

$$(H_{Atomic} + V_{Interaction}) = \sum_{i=1}^{N} u_i |i> = E \sum_{i=1}^{N} u_i |i> \qquad \ldots(6)$$

Projecting out using $<j|$ produce

$$E_i u_i + \sum_{i=1}^{N} u_i <j| V_{Interaction}|i> = E u_j \qquad \ldots(7)$$

2. Methodology

In this study we are interested in utilizing the LCAO Workbench computational tool to interactively alter the atomic parameters in order to visualize the resulting atomic cluster and the produced molecular orbitals. The implemented software allows the user to treat the atoms as 2D cylindrical square-well problem, evaluates the cluster states wavefunction, and calculate the elements of the corresponding Hamiltonian matrix of a number of configurations. This section breaks down the calculation concepts and the computation procedure followed. The examined atoms in LCAO Workbench are treated as cylindrical square wells characterized by a particular radius, depth and position. Any atom is defined as

$$atomObj_i = Initialize(r_i, V_{oi}, x_i, y_i) \qquad \ldots(8)$$

each atom within the cluster will initialize by calling the $Initialize$ function which give a definite radius (r_i), depth (V_{oi}), and position (x_i, y_i). The radii influence the manner in which the wave functions are determined, as they considered the extent over which the electron's probability density exists. On the other hand, the potential well depth values

control the orbital energy levels of the electron. In general, the potential energy of any atom ($atomObj_i$) is defined as

$$V(r_i) = \begin{Bmatrix} -V_o & if & r_i \le R \\ 0 & if & r_i > R \end{Bmatrix} \quad \ldots(9)$$

for R being the general or reference radius. Finally, the positions of the atoms are crucial in evaluating each element in the Hamiltonian matrix as well as visualizing the atoms. For an electron confined in the potential well, the wavefunction $\psi(r)$ is simply the solution of Equation (2). Bessel function of the first kind represent the wavefunction inside the potential well. In contrast, the wavefuction outside the potential well is defined by Bessel function of the second kind. Generally, in the event that $r_i \le R$, the wave function is represented by:

$$\psi_{in}(r) = \mathcal{A} J_m(\alpha r) \quad \ldots(10)$$

where the relationship between the momentum quantum number m, the wave number, and the energy E is

$$\alpha = \sqrt{\frac{2m_e(E + V_o)}{\hbar^2}} \quad \ldots(11)$$

Outside the well where the condition $r_i > R$ is satisfied, the wavefunction $\psi_{out}(r)$ is related to the modified Bessel function of the second kind K_m

$$\psi_{out}(r) = \mathcal{B} K_m(\beta r) \quad \ldots(12)$$

the constant β pertinent to the energy as

$$\beta = \sqrt{\frac{2m_e(-V_o)}{\hbar^2}} \quad \ldots(13)$$

Employing the boundary condition ($r = R$), the two unknown coefficients $\mathcal{A}$ and $\mathcal{B}$ can be readily ascertained using

$$\left.\frac{d\psi_{in}(r)}{dr}\right|_{r=R} = \left.\frac{d\psi_{out}(r)}{dr}\right|_{r=R} \quad \ldots(14)$$

$$\int_0^\infty 2\pi|\psi(r)|^2 r dr = 1 \quad \ldots(15)$$

$$\begin{cases} \int_0^R 2\pi\mathcal{A}^2|J_m(\alpha r)|^2 r dr, & r < R \\ \int_R^\infty 2\pi\mathcal{B}^2|K_m(\beta r)|^2 r dr, & r \ge R \end{cases} \quad \ldots(16)$$

the above normalization condition must be strictly satisfied, the utilizing code has a normalizing procedure named 'Normalize' which altering the coefficients $\mathcal{A}$ and $\mathcal{B}$ appropriately. By solving Equation (2), the energy eigenvalues can be ascertained. In fact, the eigenvalues are derived by identifying the roots of Equation (12) that derived from the boundary condition ($r = R$) . This is accomplished computationally in the '*FindEnergy*' procedure using an algorithm for root-finding technique. In order to guarantee a non-trivial solution of the wavefunction, the determinant of the coefficients $\mathcal{A}$ and $\mathcal{B}$ must set to be zero. As a consequence, the eigenvalue equation can be solved to end up with the required energy value.

$$\begin{vmatrix} J_m(\alpha r) & -K_m(\beta r) \\ \alpha \left.\frac{dJ_m(\alpha r)}{dr}\right|_{r=R} & -\beta \left.\frac{dK_m(\beta r)}{dr}\right|_{r=R} \end{vmatrix} = 0 \quad \ldots(17)$$

The permissible energy levels are determined by solving the above equation for E. To refine the energy eigenvalues iteratively, we implement the following equation

$$E = \frac{1}{depth}\left(-\frac{\hbar^2 k^2}{2m}\right) \quad \ldots(18)$$

It is vital to mention here that the two Bessel functions are crucial and extensively used in evaluating the radial part of the Schrödinger equation. For the sake of efficient and precise calculation the following recursion equations are utilized:

$$J_{m+1}(r) = \frac{2m}{r} J_m(r) - J_{m-1}(r)$$
$$K_{m+1}(r) = \frac{2m}{r} k_m(r) + K_{m-1}(r) \quad \ldots(19)$$

The code incorporates procedures for estimating these functions, taking into account both direct calculation and interpolation from precomputed values.

If an atomic cluster is formed and $\psi_i(r)$ and $\psi_j(r)$ are the wavefunctions of the two atoms, and $V(r)$ is the interaction potential then, the matrix element in the form of integration is given by

$$\langle i|V_{Interaction}|j\rangle = \int_0^\infty \psi_i(r) V(r) \psi_j(r) \frac{dr}{2\pi r} \quad \ldots(20)$$

In the used code, the value of this integral is estimated by Simpson's rule for numerical integration (Cune, 2007).

3. Construction of Hamiltonian Matrix

An atomic cluster of N atomic quantum states, the Hamiltonian matrix (H_{ij}) is commonly a matrix of order $N \times N$, depicts the atomic interaction (between i-th and j-th atomic quantum states) within a system of atoms. Within the H_{ij} matrix, two main types of elements are distinguishable; on the absence of interaction between atoms of the system at hands, the diagonal elements describes the on-site-energies (H_{ii}), while the rest correspond to the interaction energies ($H_{ij}\big|_{i\neq j}$). The diagonal on-site-energies are merely the isolated atom's energy ($H_{ii} = E_i|_{iso}$) and the interaction energies are estimated according to the following

$$H_{ij} = \langle i|V_{Interaction}|j\rangle \quad \ldots(21)$$

$$H_{ij} = \int \psi_i^*(\boldsymbol{r})\, V_{Interaction}(\boldsymbol{r}) \psi_j(\boldsymbol{r}) d(\boldsymbol{r}) \quad \ldots(22)$$

in this context $\boldsymbol{r}$ refers to the spatial coordinates. In the implemented code this calculation is curried out within the '*MatrixElement*' procedure. This procedure calculates the above mentioned matrix elements by considering the central distance between any pair of atoms with respect to the associated wavefunctions and the potential depth. Typically, for instance, a cluster composed of N atoms the constructed Hamiltonian matrix will be

$$H = \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & \cdots & H_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & \cdots & H_{NN} \end{pmatrix} \quad \ldots(23)$$

In order to evaluate the values of the energy levels, the Hamiltonian matrix should be diagonalized. Specifically, the used code executes the diagonalization process via two base steps; first with the aid of Householder transformation the Hamiltonian matrix reduced to a tridiagonal form, subsequently applying the QL algorithm[3] to estimate the eigenvectors and the corresponding eigenvalues (Noble, 2017). A defined variable within the implemented code named 'whichState' allows the user to select one of the calculated eigenstates for focusing purposes, further investigation and subsequent calculation. For the purpose of cluster's wavefunction formulation the used code sums all the contributions from the combined atoms in the selected eigenstate.

4. Results and Discussion

4.1 Quantum Visualization of a Homo-Diatomic Molecule

To examine a system composed of two identical atoms, we defined the radius and the distance between the atoms prior to running the code. The used code allows the user to investigate a range of atomic radii varying from 0.5 to 10 measured in arbitrary units; on the other hand, the well depth domain is ranges from 0.1 to 10. The two atoms are laying on the x-axis and the (x_i, y_i) are defined, the radius of each atom and the well depth are 2 and 1 respectively. Figure (1) depicts the atomic cluster, the energy levels for the cluster-stat wavefunction at the energy of interest (-0.14), the specific cluster-state wavefunction, and the wavefunction of the selected atom (placed at the origin). Figure (1-a) shows a simple system of two identical atoms positioned along the horizontal axis with a relatively notable distance between them. Energy Levels of the Cluster-State wavefunction is illustrated in Figure (1-b); this plot exhibits the energy levels corresponding to the '*bonding'* and '*antibonding'* states of the homo-diatomic molecule system as a function of interatomic distance. Owing to the remarkable distance between atoms, a narrow gap between energy levels has been noted (demonstrates poor bounding interaction). The particular cluster-state wavefunction exhibits the spatial distribution of electron probability density arising from the interaction of atomic wavefunctions (Figure (1-c)). The equilibrated form of the wavefunction, emphasized by contour lines, indicates constructive interference, creating a delocalized bonding state. The electron cloud's utmost probability density ($\emptyset \approx 0.1$) is confined to the bonding region, highlighting the critical overlap of wavefunctions. this behavior exemplifies the core mechanism by which atomic wavefunctions merge to create molecular orbitals, immediately affecting electronic transport properties in materials. The visualization reveals key perspectives on bonding phenomena in atomic clusters, harmonizing with established theoretical schemas in quantum mechanics and material science (Cramer, 2013). The graphical representation of the wavefunction for the atom at the reference point, as shown in Figure (1-d), reveals perspectives on the particularized character of the electron in the

[3] The QL algorithm is a numerical procedure implemented to evaluate the eigenvalues and eigenvectors of a symmetric tridiagonal matrices. It proficiently iterates by means of orthogonal transformations, strongly associated with the QL algorithm, to simplify the matrix into diagonal form.

potential well. The wavefunction displays peak magnitude of approximately $\emptyset(0) = 0.1$ at the origin and declines following an exponential function with increasing radial distance. This behavior is in line with the solution of the Schrödinger equation (Equation 2), where the radial part of the wavefunction within the well is depicted by the Bessel function of the first kind, and outside the well with the revised Bessel function of the second kind. Beyond the atomic border, the quick attenuation of the wavefunction highlights the restriction of the electron inside the well-defined potential. The exponential decline revealed in the diagram indicates the distinguishing behavior of bound states, with the confinement principally determined by the potential well depth and radius. This graphical representation supports the theoretical predictions of cylindrical square-well potentials and highlights the character of wavefunction localization in defining atomic and electronic properties within clusters.

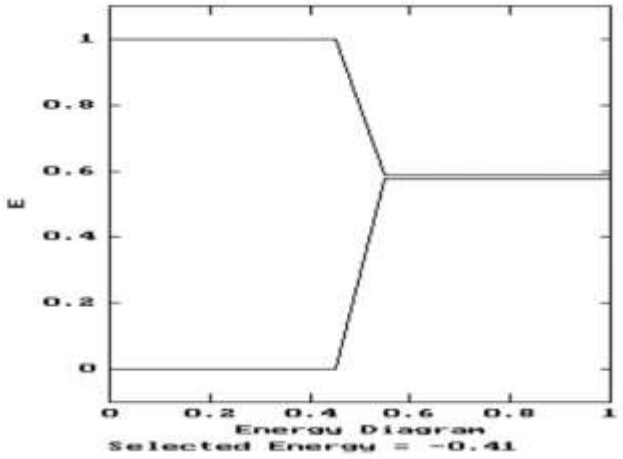

Figure 1-a: An atomic cluster consisting of two identical atoms that are relatively far apart from each other.

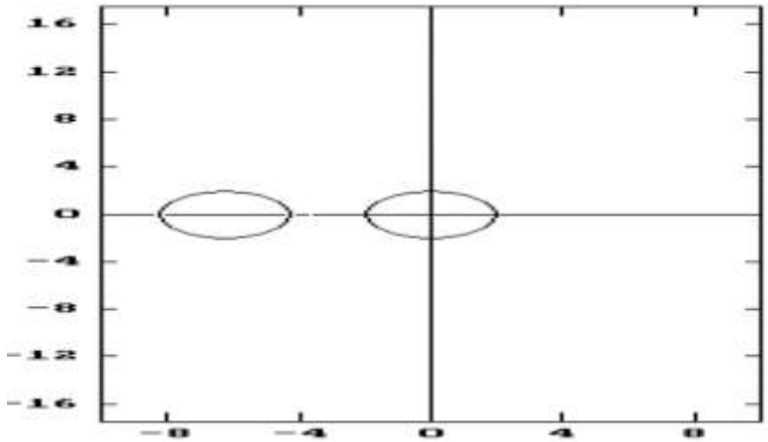

Figure 2-b: The energy levels for the cluster-state wavefunction at the energy of interest.

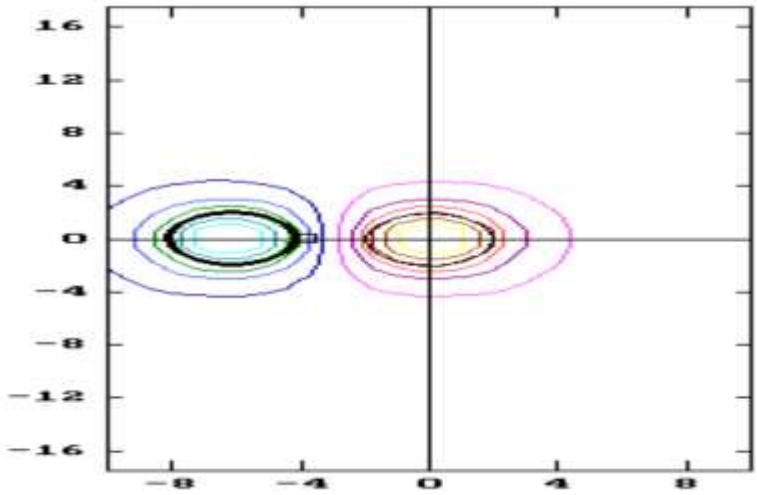

Figure 3-c: The specific cluster-state wavefunction.

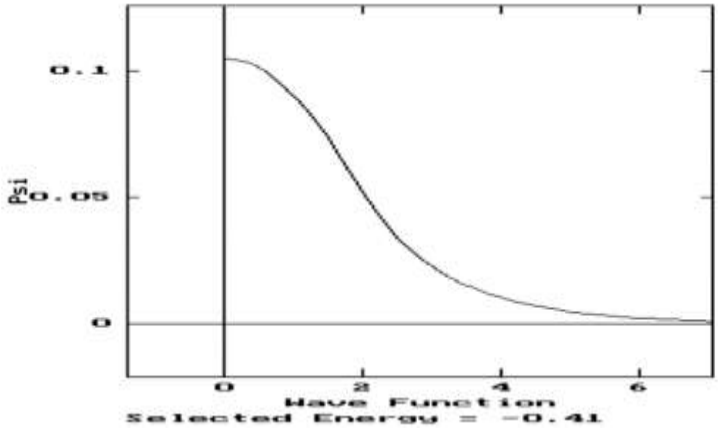

Figure 4-d: The wavefunction of the selected atom (the atom at the origin).

Figure 5: Quantum mechanical visualization of an atomic-cluster consisting of two identical atoms: energy level distributions, probability densities, and wave function aspects.

4.2 Quantum Visualization of a Hetero-Diatomic Molecule

Broadening the analysis from the Homo-Diatomic Molecule, this research also explores a Hetero-Diatomic Molecule with two atoms differing in dimensions and potential. The smaller atom at the reference point (radius = 2, well depth = 1) and a larger adjacent atom (radius = 4, well depth = 1) present asymmetry that meaningfully impacts bonding and antibonding states (as depicted in Figure 2). For the upper energy state ($E \approx -0.24$), presented in Figure (2-b), destructive interference gives rise to an antibonding configuration with diminished wavefunction overlap. This yields substantial electron delocalization headed for the larger-sized atom. Whereas, the lower energy state ($E \approx -0.77$), illustrated in Figure (2-d), reveals a bonding configuration characterized by symmetric electron density between the atoms (Figure 2-c). In comparison to the symmetric Homo-Diatomic Molecule, the Hetero-Diatomic System indicates substantial differences in bonding behavior, underscoring the role of atomic scale and potential

on molecular stability. These results correspond with previous studies on the influence of asymmetry in molding electronic and bonding characteristics (Zhu, 2011). It is remarkable to mention that at the selected energy ($E \approx -0.24$), the contour plot illustrations the electron probability density with colored rings demonstrating regions of constant $|\varphi|^2$ values. The central rings are concerted around the atom of small radius, signifying robust electron localization due to its smaller radius and enhanced confinement (Figure 2-a). The outer rings expand in the direction of the larger atom, reflecting partial wavefunction delocalization affected by the larger atom's weaker potential. The transition in color from warm to cool signifies the exponential decay of the wavefunction with distance. This asymmetry emphasizes the interdependence between atomic size and potential in shaping the electron's spatial configuration. On the other hand, contour plot aligns with the stable bonding state, as demonstrated in the energy diagram is shown in Figures 2-c and d. The electron probability density is wholly localized around the atom of large radius, with inner contours demonstrating high-concentration confinement and outer contours manifesting elongation towards lower-density regions. This denotes considerable wavefunction overlap and constructive interference, characteristic of a bonding molecular orbital. The smaller atom's influence is negligible, stress the dominant role of the larger atom in determining the wavefunction.

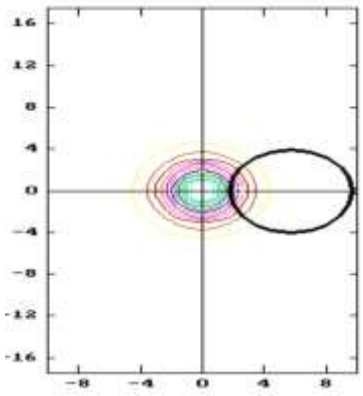

Figure 2-a: An atomic cluster consisting of two Distinct atoms that are relatively close to each other with atom at the origin being smaller than the adjacent atom.

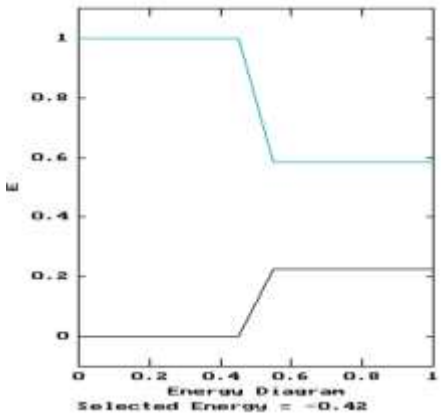

Figure 2-b: Energy levels for the upper energy state ($E \approx -0.42$).

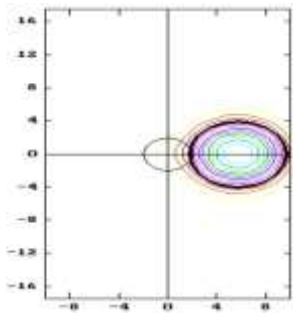

Figure 2-c: The specific cluster-state wavefunction of the selected energy line.

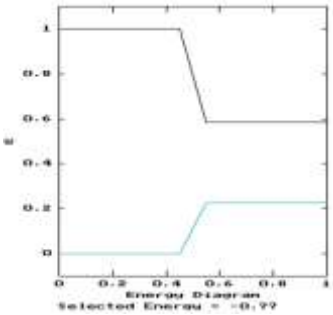

Figure 2-d: Energy levels for the upper energy state ($E \approx -0.77$).

Figure: 2 Quantum mechanical visualization of a hetero-diatomic molecule

5. Conclusion

This research employed the Linear Combination of Atomic Orbitals (LCAO) method to simulate and examine the quantum mechanical behavior of Homo- and Hetero-Diatomic Molecules. The assessment of Homo-Diatomic Systems elucidated symmetric bonding and antibonding states as a result of equal atomic radii and potentials, causing closely spaced energy levels and balanced wavefunction distributions. conversely, the Hetero-Diatomic Molecule proved pronounced asymmetry, with the atom of high radius dominating the wavefunction localization in both bonding and antibonding states. The bonding state of the Hetero-Diatomic Molecule displayed robust wavefunction overlap and constructive interference, giving rise to a stable molecular orbital with a lower energy ($E \approx -0.77$). On the contrary the antibonding state exhibited minimal overlap and electron delocalization in the direction of the larger atom, yielding a higher energy state ($E \approx -0.24$). These results highlight the decisive impact of atomic dimension and potential on molecular stability, with atoms of high radius playing a dominant role in shaping the electronic structure and energy distribution. This research demonstrates the flexibility of the LCAO approach in modeling complex atomic interactions and offers significant understanding of the electronic properties of atomic clusters. The findings concur with theoretical expectations, accentuating the significance of wavefunction localization and interference in assessing molecular stability and energy levels, and presenting a schema for future exploration of nanoscale quantum systems (Evarestov, 2012), (Kanada-En'yo, 2021) and (Wang, 2024).

References

Cardona, M. F. (2007). Quantum Chemistry of Solids: The LCAO First Principles Treatment of Crystals. Berlin: Springer.

Cramer, C. J. (2013). Essentials of computational chemistry: theories and models. John Wiley & Sons.

Cune, L. C. (2007). Atomic clusters and nanostructures. *Digest Journal of Nanomaterials and Biostructures*, 2(4), 315-333.

Evarestov, R. A. (2012). *Quantum chemistry of solids: LCAO treatment of crystals and*

nanostructures. Heidelberg: Springer Berlin Heidelberg.

Kanada-En'yo, Y., & Lee, D. (2021). Effective interactions between nuclear clusters. *Physical Review C*, *103*(2), 024318.

Noble, J. H. (2017). Diagonalization of complex symmetric matrices: Generalized Householder reflections, iterative deflation and implicit shifts. *Computer Physics Communications*, 221, 304-316.

Pal, R. P. (2021). Atomic clusters: Structure, reactivity, bonding, and dynamics. *Frontiers in Chemistry*, 9, 730548.

Silsbee, R. H. (1997). *Simulations for Solid State Physics Hardback with CD-ROM: An Interactive Resource for Students and Teachers. CUP Archive.*

Slater, J. C. (1954). Simplified LCAO method for the periodic potential problem. *Physical review*, 94(6), 1498.

Wang, Z. Y. (2024). Selecting dual atomic clusters supported on two-dimensional biphenylene with significantly optimized capability to reduce carbon monoxide. *Journal of Materials Chemistry A*, 12(5), 2748-2759.

Zhu, X. Z. (2011). Two-center interference in high-order harmonic generation from heteronuclear diatomic molecules. *Optics express*, 19(2), 436-447.