Supporting Information for

Density Functional Calculations on H_2 Using 1s Slater Type Orbitals

Choirun Nisaa Rangkuti[1], Suci Faniandari[1], A Suparmi[2] and Yanoar Pribadi Sarwono[1*]

[1]Research Center for Quantum Physics, National Research and Innovation Agency (BRIN), South Tangerang 15314, Indonesia

[2]Department of Physics, Faculty of Mathematics and Natural Sciences, Universitas Sebelas Maret, 57126, Indonesia

E-mail: yano001@brin.go.id

1. Installation instructions

1. Open Google Collaboratory https://colab.research.google.com/ and log in with Google username and password. Then, you will be prompted to the welcome screen shown in the figure
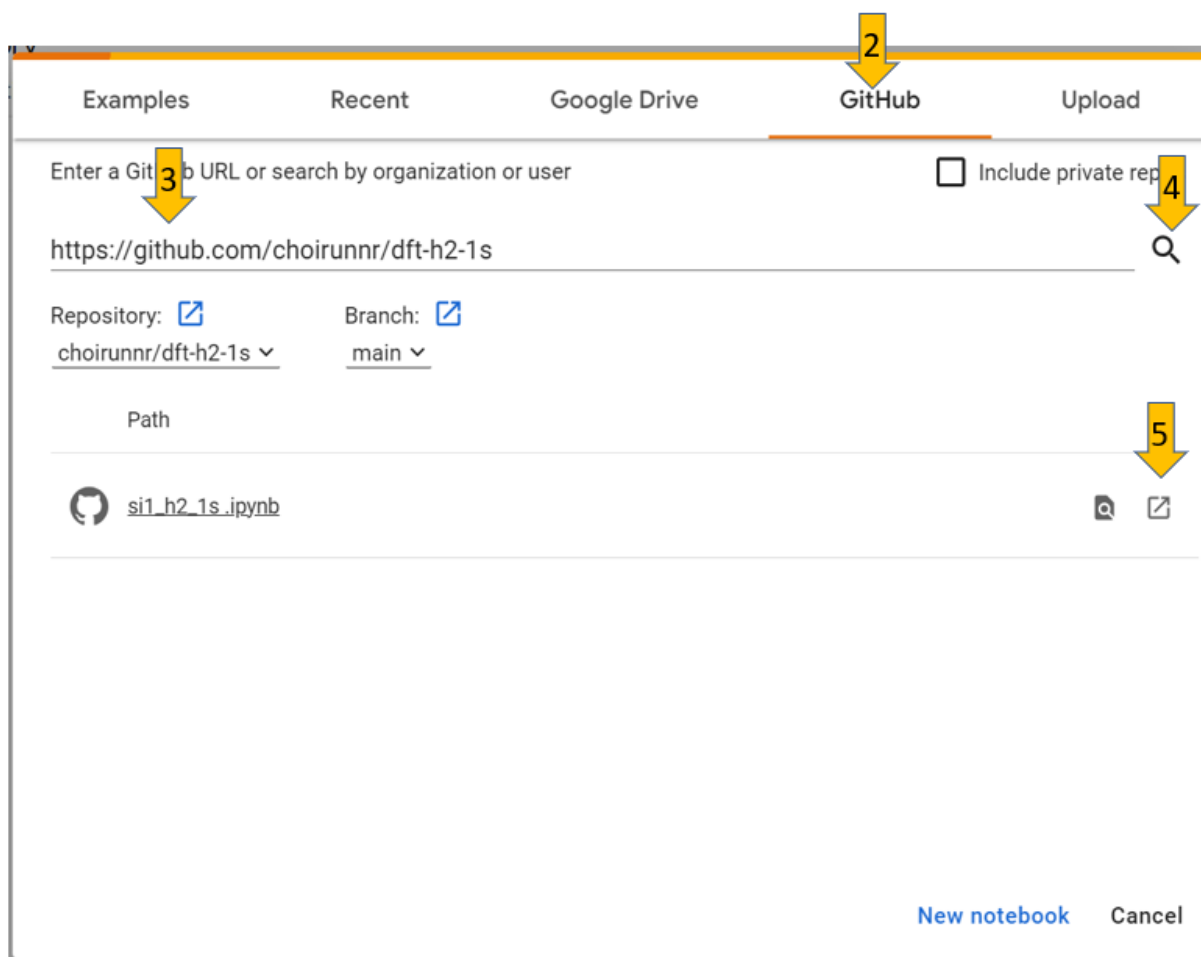
2. Choose the GitHub tab

3. At "Enter a GitHub URL or search by organization or user", type this GitHub address: https://github.com/choirunnr/dft-h2-1s

4. Click the search button

5. Choose "Open notebook in a new tab"

2. Fundamental integrals of the H₂ involving the 1s STOs

2.1. The fundamental integrals of the H_2 to calculate the kinetic, the ionic, and the Hartree energy of the H_2 [1, 2]

Table 1 Ten integrals of the H_2 molecule

Integral	Expression	Description	Value
I_1	$\langle a(\mathbf{r}) \vert b(\mathbf{r}) \rangle$	Overlap integral	S
I_2	$\langle a(\mathbf{r}) \vert -\frac{1}{2}\nabla^2 \vert a(\mathbf{r}) \rangle$	Kinetic energy of electron centered on nucleus a	$\alpha^2/2$
I_3	$\langle a(\mathbf{r}) \vert -\frac{1}{2}\nabla^2 \vert b(\mathbf{r}) \rangle$	Exchange kinetic energy of electron	$-\alpha^2(K+S/2)$
I_4	$\langle a(\mathbf{r}) \vert -\frac{1}{r_{1a}} \vert a(\mathbf{r}) \rangle$	Coulomb attraction of electron centered on nucleus a to nucleus a	$-\alpha$
I_5	$\langle a(\mathbf{r}) \vert -\frac{1}{r_{1b}} \vert a(\mathbf{r}) \rangle$	Coulomb attraction of electron centered on nucleus a to nucleus b	αJ
I_6	$\langle a(\mathbf{r}) \vert -\frac{1}{r_{1a}} \vert b(\mathbf{r}) \rangle$	Exchange Coulomb electron-nucleus attraction energy	αK
I_7	$\langle a(\mathbf{r}_1)b(\mathbf{r}_2) \vert \frac{1}{r_{12}} \vert a(\mathbf{r}_1)b(\mathbf{r}_2) \rangle$	Coulomb repulsion of electron 1 centered on nucleus a and electron 2 centered on nucleus b	$\alpha J'$
I_8	$\langle a(\mathbf{r}_1)b(\mathbf{r}_2) \vert \frac{1}{r_{12}} \vert b(\mathbf{r}_1)a(\mathbf{r}_2) \rangle$	Exchange Coulomb electron repulsion energy	$\alpha K'$

I_9	$\langle a(\mathbf{r}_1)a(\mathbf{r}_2)\|\frac{1}{r_{12}}\|a(\mathbf{r}_1)a(\mathbf{r}_2)\rangle$	Coulomb repulsion of electron 1 centered on nucleus a and electron 2 centered on nucleus a	$5\alpha/8$
I_{10}	$\langle a(\mathbf{r}_1)a(\mathbf{r}_2)\|\frac{1}{r_{12}}\|a(\mathbf{r}_1)b(\mathbf{r}_2)\rangle$	Exchange Coulomb electron repulsion energy	αL

Table 2 Expression of the *w*-dependence of the fundamental integrals, where $w = \alpha R$

Integrals	Expression
S	$e^{-w}\left(1 + w + \dfrac{1}{3}w^2\right)$
S'	$e^{-w}\left(1 - w + \dfrac{1}{3}w^2\right)$
J	$-\dfrac{1}{w} + e^{-2w}\left(1 + \dfrac{1}{w}\right)$
K	$-e^{-w}(1 + w)$
J'	$\dfrac{1}{w} - e^{-2w}\left(\dfrac{1}{w} + \dfrac{11}{8} + \dfrac{3w}{4} + \dfrac{w^2}{6}\right)$
K'	$\dfrac{1}{5}\left\{ e^{-2w}\left(-\dfrac{25}{8} + \dfrac{23w}{4} + 3w^2 + \dfrac{w^3}{3}\right) + \dfrac{6}{w}\left[S^2(\gamma + \ln w) + S'^2\, E_i(-4w) - 2SS'\, E_i(-2w)\right]\right\}$
L	$e^{-w}\left(w + \dfrac{1}{8} + \dfrac{5}{16w}\right) + e^{-3w}\left(-\dfrac{1}{8} - \dfrac{5}{16w}\right)$
C	Euler's constant $= 0.57722$
$E_i(x)$	Integral logarithm, $E_i(-x) = -\displaystyle\int_x^{\infty} \dfrac{e^{-t}}{t}\,dt,\ x > 0$

2.2. The involved symmetries with the explanations to evaluate the Hartree energy

Table 3 The integrals for evaluating the Hartree energy

No	Integrals	Results	Remarks
1	$\langle ab'|g|ba'\rangle$		From Table 1
2.	$\langle aa'|g|bb'\rangle$	$\alpha K'$	Swap $j \leftrightarrow l$ for $\langle ij|g|kl\rangle$

3.	$\langle ba'\vert g\vert ab'\rangle$		Swap $b\leftrightarrow a$
4.	$\langle bb'\vert g\vert aa'\rangle$		Swap $i\leftrightarrow k$ for $\langle ij\vert g\vert kl\rangle$ then use No. 1
5.	$\langle ab'\vert g\vert ab'\rangle$		From Table 1
6.	$\langle ba'\vert g\vert ba'\rangle$	$\alpha J'$	Swap $b\leftrightarrow a$
7.	$\langle aa'\vert g\vert ab'\rangle$		From Table 1
8.	$\langle aa'\vert g\vert ba'\rangle$		
9.	$\langle ab'\vert g\vert aa'\rangle$		
10.	$\langle ab'\vert g\vert bb'\rangle$		Either from symmetry or changing $b\leftrightarrow a$, for example:
11.	$\langle ba'\vert g\vert aa'\rangle$	αL	
12.	$\langle ba'\vert g\vert bb'\rangle$		$\langle aa'\vert g\vert ba'\rangle\overset{\text{swap the coordinate (')}}{=}\langle a'a\vert g\vert b'a\rangle$
13.	$\langle bb'\vert g\vert ab'\rangle$		$\overset{\text{permutate}}{=}\langle aa'\vert g\vert ab'\rangle$
14.	$\langle bb'\vert g\vert ba'\rangle$		
15.	$\langle aa'\vert g\vert aa'\rangle$		From Table 1
16.	$\langle bb'\vert g\vert bb'\rangle$	$5\alpha/8$	

3. Activities 1-5

3.1. Activity 1: Construction of the density of the H₂ using the 1s orbitals

The hydrogen molecule H_2 is illustrated with the cartoon sketch Fig. 1. The numbers 1 and 2 represent the first and second electron, while the label a and b denote the two nuclei of the hydrogen atoms. The density functional theory (DFT) calculation is started with the construction of a "one-electron" wave function shown with the red dashed line. From the main text (here Eq. (1)), the molecular orbital $\psi_1(\mathbf{r})$ is constructed from the sum of two 1s orbitals centered at nucleus a, $a(\mathbf{r})$ and b, $b(\mathbf{r})$

$$\psi_1(\mathbf{r}) = \frac{1}{\sqrt{2(1+S)}}\left(a(\mathbf{r})+b(\mathbf{r})\right). \tag{1}$$
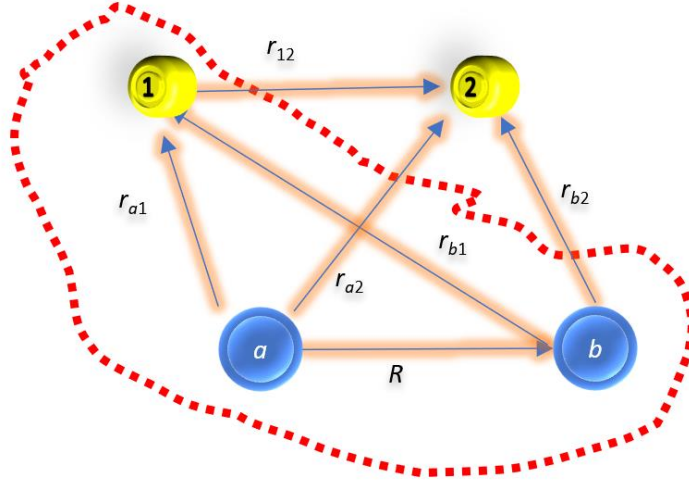

Fig. 1 The cartoon sketch of the H_2

The explicit expression of the overlap integral S is shown in Table 6 Appendix A. The $1s$ orbital centered at a, $a(\mathbf{r})$ has the form of

$$a(\mathbf{r}) = \sqrt{\frac{\alpha^3}{\pi}}e^{-\alpha r_a}. \tag{2}$$

The value of the orbital exponent α is set as 1.24, corresponding to the parameters used in the STO-3G and the STO-6G basis set[3] Eq. (1) illustrates the concept of the linear combination of atomic orbitals LCAO[4] in the construction of the molecular orbital. After forming the molecular orbital, we may calculate the density n, with the factor of 2 corresponding to the number of electrons

$$\begin{aligned}
n(\mathbf{r}) &= 2\times|\psi_1(\mathbf{r})|^2 \\
&= 2\times\frac{1}{2(1+S)}\left(a(\mathbf{r})+b(\mathbf{r})\right)^2 \\
&= \frac{\alpha^3}{\pi(1+S)}\left(e^{-\alpha r_a}+e^{-\alpha r_b}\right)^2.
\end{aligned} \tag{3}$$

The last step is obtained by substituting the expression of $a(\mathbf{r})$ Eq. (2).

Questions:

1. What is the linear combination of atomic orbital LCAO? Using $1s$ orbitals centered at nucleus a and b, $a(\mathbf{r})$ and $b(\mathbf{r})$, construct the one-electron molecular orbital of the H_2.

2. What is the density of the H_2 given the molecular orbital Eq. (1)?

3.2. Activity 2: Calculation of the kinetic and the ionic energy of the H_2

The evaluation of the total kinetic energy $E_T[n]$ is as follows

$$E_T[n] = 2\left\langle \psi_1(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 \right| \psi_1(\mathbf{r}) \right\rangle, \tag{4}$$

Where the factor of 2 corresponds to the number of electrons. Substitution Eq. (1) into Eq. (4) and expansion the terms lead to

$$
\begin{aligned}
E_T[n] &= \frac{1}{(1+S)}\left\langle a(\mathbf{r})+b(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 \right| a(\mathbf{r})+b(\mathbf{r}) \right\rangle \\
&= \frac{1}{(1+S)}\left[
\begin{array}{l}
\left\langle a(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 \right| a(\mathbf{r}) \right\rangle + \left\langle a(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 \right| b(\mathbf{r}) \right\rangle + \\
\left\langle b(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 \right| a(\mathbf{r}) \right\rangle + \left\langle b(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 \right| b(\mathbf{r}) \right\rangle
\end{array}
\right].
\end{aligned}
\tag{5}
$$

Consulting the Table 5 Appendix A, we get

$$
\begin{aligned}
E_T[n] &= \frac{1}{(1+S)}\left[
\begin{array}{l}
\frac{\alpha^2}{2} - \alpha^2\left(K+\frac{S}{2}\right) \\
-\alpha^2\left(K+\frac{S}{2}\right)+\frac{\alpha^2}{2}
\end{array}
\right] \\
&= \frac{\alpha^2}{(1+S)}\left[1-2K-S\right].
\end{aligned}
\tag{6}
$$

Using the similar steps, we get the total ionic energy $E_V[n]$

$$E_V[n] = 2\left\langle \psi_1(\mathbf{r})\left|-\frac{1}{r_a}-\frac{1}{r_b}\right|\psi_1(\mathbf{r})\right\rangle. \tag{7}$$

Expanding Eq. (7) with the expression of the $\psi_1(\mathbf{r})$, we get

$$E_V[n] = \frac{1}{(1+S)}\left\langle a(\mathbf{r})+b(\mathbf{r})\left|-\frac{1}{r_a}-\frac{1}{r_b}\right|a(\mathbf{r})+b(\mathbf{r})\right\rangle$$

$$= \frac{1}{(1+S)}\left[\begin{array}{l}\left\langle a(\mathbf{r})\left|-\frac{1}{r_a}\right|a(\mathbf{r})\right\rangle+\left\langle a(\mathbf{r})\left|-\frac{1}{r_a}\right|b(\mathbf{r})\right\rangle+\left\langle b(\mathbf{r})\left|-\frac{1}{r_a}\right|a(\mathbf{r})\right\rangle+\left\langle b(\mathbf{r})\left|-\frac{1}{r_a}\right|b(\mathbf{r})\right\rangle+\\ \left\langle a(\mathbf{r})\left|-\frac{1}{r_b}\right|a(\mathbf{r})\right\rangle+\left\langle a(\mathbf{r})\left|-\frac{1}{r_b}\right|b(\mathbf{r})\right\rangle+\left\langle b(\mathbf{r})\left|-\frac{1}{r_b}\right|a(\mathbf{r})\right\rangle+\left\langle b(\mathbf{r})\left|-\frac{1}{r_b}\right|b(\mathbf{r})\right\rangle\end{array}\right]. \tag{8}$$

Consulting the Table 5 Appendix A, we get

$$E_V[n] = \frac{1}{(1+S)}\left[\begin{array}{l}-\alpha+\alpha K+\alpha K+\alpha J+\\ \alpha J+\alpha K+\alpha K-\alpha\end{array}\right]$$

$$= \frac{2\alpha}{(1+S)}[-1+J+2K]. \tag{9}$$

Questions

1. Using the Table 5 Appendix A, what is the expression of the one-electron kinetic energy $E_T[n]$ of the H$_2$ given the molecular orbital $\psi_1(\mathbf{r})$ Eq. (1) in terms of α, K, S?

2. What is the expression of the one-electron ionic energy $E_V[n]$ of the H$_2$ given the molecular orbital $\psi_1(\mathbf{r})$ Eq. (1) in terms of α, J, K, S?

3.3. Activity 3: Calculation of the Hartree energy of the H$_2$ using 1s orbitals

The evaluation of the Hartree energy $E_J[n]$ is not as straightforward as the previous energies because of additional terms and the involved symmetries. The $E_J[n]$ is defined as follows

$$E_J[n] = 2\left\langle \psi_1(\mathbf{r})\psi_1(\mathbf{r}') \Big| \frac{1}{|\mathbf{r}-\mathbf{r}'|} \Big| \psi_1(\mathbf{r})\psi_1(\mathbf{r}') \right\rangle$$

$$= 2\left(\frac{1}{2(1+S)}\right)^2 \left\langle (a(\mathbf{r})+b(\mathbf{r}))(a(\mathbf{r}')+b(\mathbf{r}')) \Big| \frac{1}{|\mathbf{r}-\mathbf{r}'|} \Big| (a(\mathbf{r})+b(\mathbf{r}))(a(\mathbf{r}')+b(\mathbf{r}')) \right\rangle.$$

(10)

To simplify the notation Eq. (10), we denote $g = \dfrac{1}{|\mathbf{r}-\mathbf{r}'|}$, $a = a(\mathbf{r})$, and $a' = a(\mathbf{r}')$,

$$E_J[n] = 2\left(\frac{1}{2(1+S)}\right)^2 \begin{bmatrix} \langle aa'|g|aa'\rangle + \langle aa'|g|ab'\rangle + \langle aa'|g|ba'\rangle + \langle aa'|g|bb'\rangle + \\ \langle ab'|g|aa'\rangle + \langle ab'|g|ab'\rangle + \langle ab'|g|ba'\rangle + \langle ab'|g|bb'\rangle + \\ \langle ba'|g|aa'\rangle + \langle ba'|g|ab'\rangle + \langle ba'|g|ba'\rangle + \langle ba'|g|bb'\rangle + \\ \langle bb'|g|aa'\rangle + \langle bb'|g|ab'\rangle + \langle bb'|g|ba'\rangle + \langle bb'|g|bb'\rangle \end{bmatrix}.$$ (11)

We can identify equivalent terms after consulting Table 7 Appendix B which provides details of the involved symmetry so that the $E_J[n]$ becomes

$$E_J[n] = 2\left(\frac{1}{2(1+S)}\right)^2 \begin{bmatrix} \dfrac{5}{8}\alpha + \alpha L + \alpha L + \alpha K' + \\ \alpha L + \alpha J' + \alpha K' + \alpha L + \\ \alpha L + \alpha K' + \alpha J' + \alpha L + \\ \alpha K' + \alpha L + \alpha L + \dfrac{5}{8}\alpha \end{bmatrix}$$

$$= \frac{1}{2(1+S)^2}\left[2\times\frac{5}{8}\alpha + 8\alpha L + 4\alpha K' + 2\alpha J'\right]$$ (12)

$$= \frac{\alpha}{(1+S)^2}\left[\frac{5}{8} + J' + 2K' + 4L\right].$$

Question

1. What is the expression of the Hartree energy $E_J[n]$ given the molecular orbital $\psi_1(\mathbf{r})$ Eq. (1) in terms of α, J', L, K', S? You may consult the Table 5 Appendix A and Table 7 Appendix B.

3.4. Activity 4: Calculation of the exchange energies of the H_2

From the main text, the exchange energy within the local density approximation (LDA) is formulated as

$$E_X = -\frac{9}{8}c\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int n(\mathbf{r})^{\frac{4}{3}}\, dV,\tag{13}$$

where $c = \frac{2}{3}$ and $c = 0.7$ give the Slater E_X^S and the X-Alpha $E_X^{X\alpha}$ exchange respectively. The exchange and correlation energy are central to the DFT because they contain all contributions that are not considered in earlier energy components. There are many available choices for the exchange and correlation. When we choose the LDA, the correlation energy $E_C[n]$ is ignored and becomes zero. This is the reason the dissociation of H_2 is not well described. The use of spin LDA[5] can describe the molecular dissociation correctly. The explicit expressions of the E_X^S and $E_X^{X\alpha}$ are

$$E_X^S = -\frac{4}{3}\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int \left(\frac{\alpha^3}{\pi(1+S)}\left(e^{-\alpha r_a}+e^{-\alpha r_b}\right)^2\right)^{\frac{4}{3}} dV$$

$$E_X^{X\alpha} = -0.7 \times \frac{9}{8}\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int \left(\frac{\alpha^3}{\pi(1+S)}\left(e^{-\alpha r_a}+e^{-\alpha r_b}\right)^2\right)^{\frac{4}{3}} dV.\tag{14}$$

In Eq. (14), the exchange energy depends on the orbital exponent α and the bond length R. Despite the integration appearing to be brief and direct, it is, in fact, quite challenging. It involves two centers, and as far as our knowledge goes, no analytical form is available. So, we need to numerically evaluate the exchange energy. The Jupyter Notebook can be used for this purpose. The integration technique we use is to express all terms in the Cartesian coordinates. While the integration using the Python library Scipy[6] is slow, other software such as Matlab or Mathematica executes the integral evaluation much faster. At the bond length R=1 bohr and the $\alpha = 1.24$, the E_X^S and $E_X^{X\alpha}$ are shown in Table 4

Table 4 The result of the Slater and X-Alpha exchange energy at the bond length R=1 bohr

Methods	Slater Exchange E_X^S	X-Alpha exchange $E_X^{X\alpha}$

STO-3G	-0.6127	-0.6433
STO-6G	-0.6129	-0.6436
$1s$	-0.6129	-0.6436

The result can be compared with calculations using standard basis sets like the STO-3G and the STO-6G. The result of the $1s$ orbital is more improved than that of the STO-3G and is approached closely by that of STO-6G.

Question:

1. What are the Slater E_X^S and the X-Alpha $E_X^{X\alpha}$ exchange energy values of H_2 at a bond length R=1.4 bohr?

3.5. Activity 5: Calculation of the DFT total energies of the H_2

In activity 5, we will calculate the total energies of the H_2 with the $1s$ orbitals. In the DFT, the total energy E_{total} is a functional of the density n. From the main text Eq. (1), the E_{total} is the sum of the energy components

$$E_{total}[n] = E_T[n] + E_V[n] + E_J[n] + E_X[n] + E_C[n], \tag{15}$$

namely the non-interacting kinetic energy functional $E_T[n]$, the ionic energy $E_V[n]$, the Hartree energy $E_J[n]$, the exchange $E_X[n]$ energy, and the correlation energy $E_C[n]$. At $R = 1$ bohr, the energy components and the total energy are shown in Table 5

Table 5 The DFT total energy and its components calculated at R=1 bohr

Methods	$E_T[n]$	$E_V[n]$	$E_J[n]$	$E_X[n]$	E_{Nuc}	E_{total}
HFS/STO-3G	1.2727	-4.0532	1.4289	-0.6127	1.0000	-0.9642
HFS/STO-6G	1.2835	-4.0739	1.4291	-0.6129	1.0000	-0.9742
HFS/$1s$	1.2837	-4.0745	1.4292	-0.6129	1.0000	-0.9745

An equivalent method to calculate the DFT total energy is to use the eigenvalue ε of the Kohn-Sham. From Eq. (2) or Eq. (6) main text, the ε is

$$2\varepsilon_1 = E_T[n] + E_V[n] + 2E_J[n] + E_X[n]. \tag{16}$$

It is easy to see that the

$$E_{total}[n] = 2\varepsilon_1 - E_J[n] + E_{Nuc} \tag{17}$$

is equivalent to the total energy Eq. (15) for the LDA exchange

$$
\begin{aligned}
E_{total}[n] &= 2\varepsilon_1 - E_J[n] + E_{Nuc} \\
&= \left(E_T[n] + E_V[n] + 2E_J[n] + E_X[n]\right) - E_J[n] + E_{Nuc} \\
&= E_T[n] + E_V[n] + E_J[n] + E_X[n]
\end{aligned} \tag{18}
$$

In Eq. (18), E_{Nuc} is a constant, not a functional of the density, under the Born-Oppenheimer approximation. We can numerically verify the equivalence of the two equations when calculating the E_{total} Eq. (15) and Eq. (17).

Questions

1. For the given table, calculate the total energy $E_{total}[n]$ of the H_2

$E_T[n]$	$E_V[n]$	$E_J[n]$	$E_X[n]$	E_{Nuc}
1.2837	-4.0745	1.4292	-0.6129	1.0000

2. Show that the E_{total} of the H_2 Eq. (17) is the same as the E_{total} with the LDA exchange?

4. Questions for Pre and Post-Test

Pre-test questions:

1. What is not included in the wavefunction-based methods to solve the Schrödinger Equation?

    A. Hartree-Fock

    B. Configuration Interaction

    C. Density functional theory

    D. Multi Configuration Self-Consistent Field

2. Using $1s$ orbitals centered at nucleus a and b, $a(\mathbf{r})$ and $b(\mathbf{r})$ respectively, what is the expression of the one-electron molecular orbital of the H_2 and its density?

    A. $a(\mathbf{r})+b(\mathbf{r})$

    B. $\left[a(\mathbf{r})-b(\mathbf{r})\right]^2$

    C. $a(\mathbf{r})b(\mathbf{r})$

    D. $\sqrt{a(\mathbf{r})+b(\mathbf{r})}$

3. For the normalization constant N, What is the expression of the density of the H_2 for the molecular orbital in question #2?

A. $N\left(a(\mathbf{r})+b(\mathbf{r})\right)$

B. $2N\left(a(\mathbf{r})+b(\mathbf{r})\right)$

C. $\left[N\left(a(\mathbf{r})+b(\mathbf{r})\right)\right]^{2}$

D. $2\left[N\left(a(\mathbf{r})+b(\mathbf{r})\right)\right]^{2}$

4. What are the energy components of the total energy based on the DFT?

    A. Kinetic, ionic, Hartree, exchange, correlation

    B. Kinetic, ionic, Hartree, exchange

    C. Kinetic, ionic, Hartree

    D. Kinetic, ionic

Post-test questions:

1.   What is not included in the wavefunction-based methods to solve the Schrödinger Equation?
    A. Hartree-Fock

    B. Configuration Interaction

    C. Density functional theory

    D. Multi Configuration Self-Consistent Field

2. Using $1s$ orbitals centered at nucleus a and b, $a(\mathbf{r})$ and $b(\mathbf{r})$ respectively, what is the expression of the one-electron molecular orbital of the H_2 and its density?

    A. $a(\mathbf{r})+b(\mathbf{r})$

    B. $\left[a(\mathbf{r})-b(\mathbf{r})\right]^{2}$

    C. $a(\mathbf{r})b(\mathbf{r})$

    D. $\sqrt{a(\mathbf{r})+b(\mathbf{r})}$

3. For the normalization constant N, What is the expression of the density of the H_2 for the molecular orbital in question #2?

    A. $N\left(a(\mathbf{r})+b(\mathbf{r})\right)$

    B. $2N\left(a(\mathbf{r})+b(\mathbf{r})\right)$

C. $\left[N\left(a(\mathbf{r})+b(\mathbf{r})\right)\right]^2$

D. $2\left[N\left(a(\mathbf{r})+b(\mathbf{r})\right)\right]^2$

4. What are the energy components of the total energy based on the DFT?

    A. Kinetic, ionic, Hartree, exchange, correlation

    B. Kinetic, ionic, Hartree, exchange

    C. Kinetic, ionic, Hartree

    D. Kinetic, ionic

5. Calculate the total energy $E_{total}[n]$ of the H_2 at R=1.4 for the given table

$E_T[n]$	$E_V[n]$	$E_J[n]$	$E_X[n]$	E_{Nuc}
1.2837	-4.0745	1.4292	-0.6129	1.0000

    A. -2.7908

    B. -1.9745

    C. -1.3616

    D. -0.9745

6. What is the possible order for the exchange energy if the basis set STO-3G, STO-6G, and 1s is respectively used?

    A. -0.6127, -0.6129, -0.6129

    B. -0.6129, -0.6127, -0.6129

    C. -0.6436, -0.6436, -0.6433

    D. -0.6436, -0.6433, -0.6436

7. Using the Table 5 Appendix A, what is the expression of the one-electron kinetic energy $E_T[n]$ of the H_2 given the molecular orbital $\psi_1(\mathbf{r})$ Eq. (1) in terms of α, K, S ?

    A. $\dfrac{\alpha^2}{(1+S)}[1-K-2S]$

    B. $\dfrac{\alpha}{(1+S)}[1-2K-S]$

    C. $\dfrac{\alpha^2}{(1+S)}[1-2K-S]$

8. What is the expression of the one-electron ionic energy $E_V[n]$ of the H_2 given the molecular orbital $\psi_1(\mathbf{r})$ Eq. (1) in terms of α, J, K, S?

A. $E_V[n] = \dfrac{2\alpha}{(1+S)}[-1 + J + 2K]$

B. $E_V[n] = \dfrac{2\alpha^2}{(1+S)}[-1 + J + 2K]$

C. $E_V[n] = \dfrac{2\alpha}{(1+S)}[-1 + 2J + K]$

9. What is the expression of the Hartree energy $E_J[n]$ given the molecular orbital $\psi_1(\mathbf{r})$ Eq. (1) in terms of α, J', L, K', S?

A. $E_J[n] = \dfrac{\alpha}{(1+S)^2}\left[\dfrac{5}{8} + J' + 2K' + 4L\right]$

B. $E_J[n] = \dfrac{\alpha^2}{(1+S)^2}\left[\dfrac{5}{8} + J' + 2K' + 4L\right]$

C. $E_J[n] = \dfrac{\alpha}{(1+S)^2}\left[\dfrac{5}{8} + 4J' + 2K' + L\right]$

10. Does the LDA DFT describe the H_2 molecular dissociation correctly?

5. Questionnaire questions

Student Questionnaires

The H_2 Jupyter Notebook

Universitas Sebelas Maret, 13 September 2023

Questionnaire: Using a scale from 1 to 5 (1=strongly disagree, 5=strongly agree), what is your level of agreement with the following statements?

	1	2	3	4	5

1. The H_2 Jupyter Notebook deepens my understanding of the DFT topic					
2. If the learning experiences are done only using a Power Point lecture, my comprehension of the DFT will not achieve the same level of understanding as that done using a Power Point lecture and the H_2 Jupyter Notebook					
3. I would like other courses to use the Jupyter Notebook such as that used in this course					
4. I can modify the H_2 Jupyter Notebook as required in the learning experiences					
5. I feel motivated to use the Jupyter Notebook for other applications and works					
Open ended questions:					
6. Three things I like about the H_2 Jupyter Notebook					
7. Three things I like the H_2 Jupyter Notebook to be improved					
8. Additional comments					

6. Gaussian input file for the (a)Slater and (b)X-Alpha Exchange energy

(a)
#P HFS/sto-6g ExtraLinks=L608 units=au

Title Card Required

```
0 1
H           -0.25000000   0.00000000   0.00000000
H            0.25000000   0.00000000   0.00000000
```

200

(b)
#P xalpha/sto-6g ExtraLinks=L608 units=au

Title Card Required

```
0 1
H            -0.25000000   0.00000000   0.00000000
H             0.25000000   0.00000000   0.00000000

300
```

7. References

1. Slater, J. C., *Quantum Theory of Molecules and Solids*. McGraw-Hill 1963.
2. Halpern, A. M.; Glendening, E. D., Exploring the Nature of the H_2 Bond. 1. Using Spreadsheet Calculations To Examine the Valence Bond and Molecular Orbital Methods. *J. Chem. Educ.* **2013,** *90* (11), 1452-1458.
3. Hehre, W. J.; Stewart, R. F.; Pople, J. A., Self‐Consistent Molecular‐Orbital Methods. I. Use of Gaussian Expansions of Slater‐Type Atomic Orbitals. *J. Chem. Phys.* **1969,** *51* (6), 2657-2664.
4. Levine, I. N., *Quantum Chemistry*. 5th ed.; Prentice Hall: Upper Saddle River, NJ, 1999.
5. Gunnarsson, O.; Lundqvist, B. I., Exchange and Correlation in Atoms, Molecules, and Solids by the Spin-Density-Functional Formalism. *Phys. Rev. B* **1976,** *13* (10), 4274-4298.
6. Virtanen, P.; Gommers, R.; Oliphant, T. E.; Haberland, M.; Reddy, T.; Cournapeau, D.; Burovski, E.; Peterson, P.; Weckesser, W.; Bright, J., SciPy 1.0: fundamental algorithms for scientific computing in Python. *Nature methods* **2020,** *17* (3), 261-272.