Interactive Graphical User Interface For Quantum Mechanics Simulations with Pyscf

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***Abstract*— This article presents a graphical user interface program developed in the Python programming language. This interface aims to make quantum mechanics simulations easier to perform using the PySCF package. paper presents a software written in Python programming language. The software offers many features to its users new opportunities on visualization, optimization, designing, and calculation for quantum mechanics and quantum gaming studies. Two explanatory examples are also implemented to show the efficiency of the interface. These examples are quantum gaming and virtual screening. Thanks to these two applications, which are frequently used in quantum mechanics simulation studies, it has been shown that the interface developed can be used effectively in both educational and research purposes.**

***Keywords*— Basis set exchange, Atomic orbitals, Gaussian-type orbitals, Quantum gaming, Quantum mechanics**

I.INTRODUCTION

Simulation tools are very useful tools for researchers and educators [1, 2]. Quantum mechanics (QM) calculations give such simulation opportunities in studying materials' properties [3]. Among these material properties, energy, geometric and band structure come first. In addition, with the increase in computing power and capacity of computers, it has become possible to predict other material properties that were previously impossible to calculate, such as piezoelectric response, photon absorption, nuclear magnetic resonance shielding and infrared Raman spectrum. Moreover, together with new and complex computational tools, it has made it possible for QM calculations to reach the accuracy of experimental measurements [4].

There are few QM methods and modeling strategies for electrons and atoms in the structure of molecules and materials in the literature. Some of these methods were developed from wave functions [5] and density functional theory [6, 7, 8]. Furthermore, QM clustering methods that take into account the specific arrangement of atoms in the structure show improvements in the speed of calculations and prediction efficiency [8]. The book, written by one the authors of this paper, gives a detailed information on QM-based simulations of models and dynamics simulations for biomolecular systems [9].

According to Atkins and Friedan [10], the time-dependent Schrödinger equation of a system is

$$ih\frac{\partial\Psi(r,t)}{\partial t} = H\Psi(r,t)$$

at the configuration of N quantum particles, $r = (r_1, r_2, \dots, r_N)$, where H is the Hamiltonian operator for the system is

$$H = -\sum_{k=1}^{N}\frac{h^2}{2m_k}\nabla_k^2 + U(r_1, r_2, \dots, r_N, t)$$

of quantum particles (with masses m_k for $k = 1,2, \dots, N$) where the terms represent the kinetic and the potential energies, respectively. Here, h is the reduced Planck's constant, $i = \sqrt{-1}$, and Ψ is the wave function describing the motion of the particles. In addition, ∇_k^2 is the operator as

$$\nabla_k^2 = \frac{\partial^2}{\partial r_k^2} = \frac{\partial^2}{\partial x_k^2} + \frac{\partial^2}{\partial y_k^2} + \frac{\partial^2}{\partial z_k^2}$$

If the potential energy (U) is independent of time, it becomes $U(r_1, r_2, \dots, r_N)$. Then, the wave-function becomes

$$\Psi(r,t) = \psi(r)T(t)$$

Then, the following time-independent Schrödinger equation can be obtained:

$$H\psi(r) = E\psi(r)$$

where H is the time-independent Hamiltonian operator and E is the energy of the particles:

$$E = \frac{\int \psi^*(\mathrm{r})H\psi(\mathrm{r})dr}{\int \psi^*(\mathrm{r})\psi(\mathrm{r})dr}$$

where * is the complex conjugate. On the other hand, $\psi^* = \psi$ if it is a real-valued function.

Pritchard and colleagues described the basis set functions of different families and a Python-based software of Basis Set

Exchange (BSE) [11]. Alternatively, Sun and colleagues presented a different Python-based simulation tool on chemistry, named PySCF [12].

II.GRAPHICAL USER INTERFACE

The Interactive Python Graphical User Interface Basis Set Exchange and Quantum Mechanics simulations using PySCF [12] software (IPySCF) is designed to enable users to perform simulations more easily. Eventually, it is an interface that filters information in the BSE database and calculates molecular properties using quantum mechanics method. Fig. 1(a) shows the main screen of the interface to the BSE data library. This screen presents interactive information query about the BSE package, content, data. There is a new feature added about the visualization of spatial orbitals for every chemical element from the periodic table. Fig. 1(b) shows that there are submenus for the related menu item.

III.FUNCTIONALITIES AND KEY FEATURES

In the following, we list key design features and their functionalities.

A. Documentation

IPySCF queries the documentation of the BSE package of Python and presents it in a readable format. That is demonstrated in Fig. 2(a) for the BSE API package and some information about the internal functions and the use of the PySCF package is shown in Fig. 2(b).

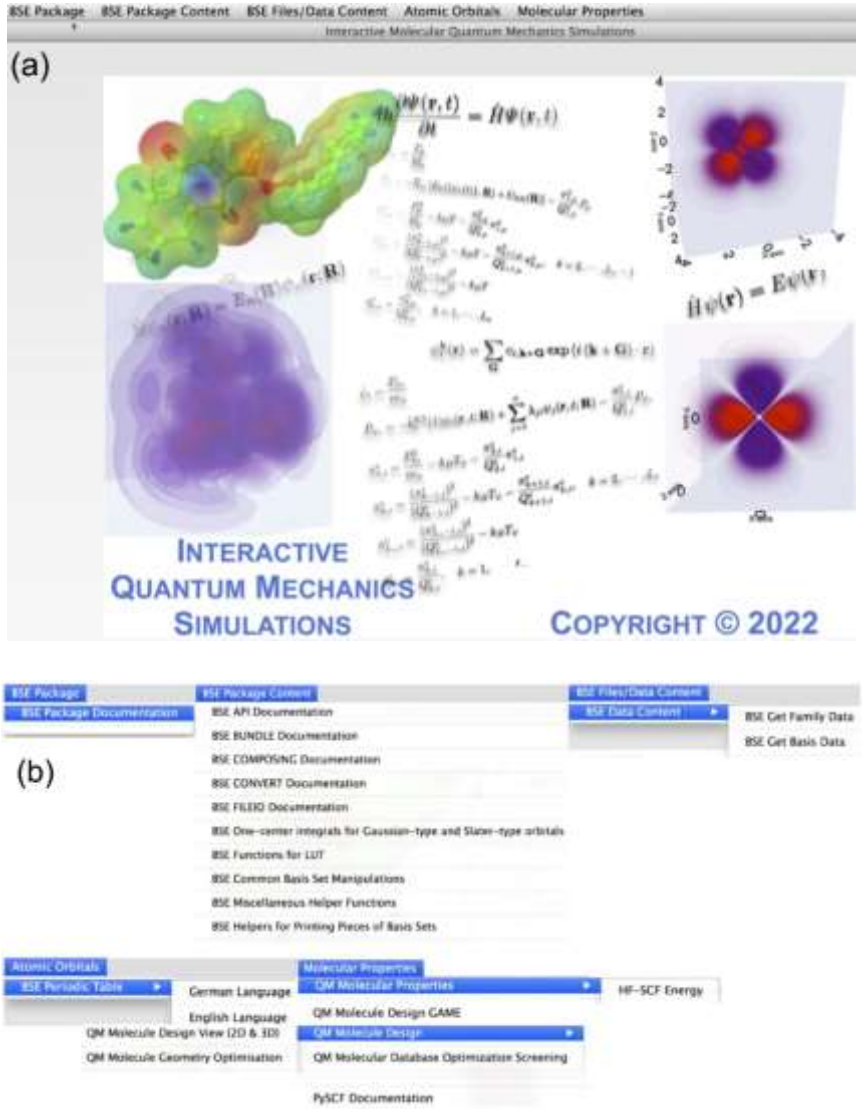

Figure 1: (a) The main screen, and (b) the menu and submenu items

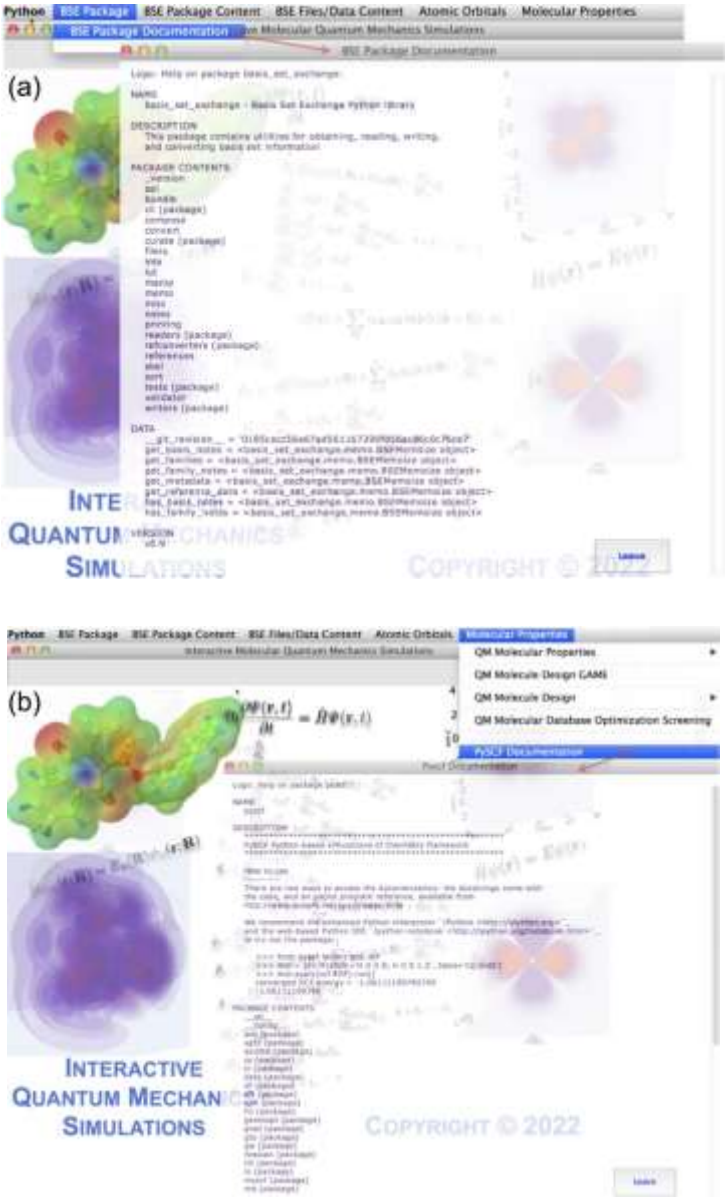

Figure 2: The documentation of (a) API package, and (b) the PySCF package

B. Query Forms

The search in the BSE database is performed through the query forms. These forms are designed as dialogues containing, for example, a Combo Box, a Check Box, and Buttons. Each of these objects has a certain functionality; for example, OK button, after clicked, leaves the dialog form, *Cancel* button destroys the dialog form, *Filter* button queries the data based on the selection from the BSE database. Fig. 3(a) presents a single query in the BSE family data. Multiple search query dialog forms are also designed. For example, Fig. 3(b) shows a double query in the BSE basis data.

C. Visualization of Atomic Orbitals

A new feature added to the current design is the visualization of atomic orbitals (AO) for each chemical element of the periodic table. In particular, every element is presented by a Button, and clicking on the chemical element from the periodic table a new window dialog appears, as shown in Fig. 4. In that window dialog, the information about the type of basis set is presented as a Combo box; the user can select one of the basis set names to apply for the current element. Next to it, there is another Combo box for choosing the format of the output information (Fig. 4).

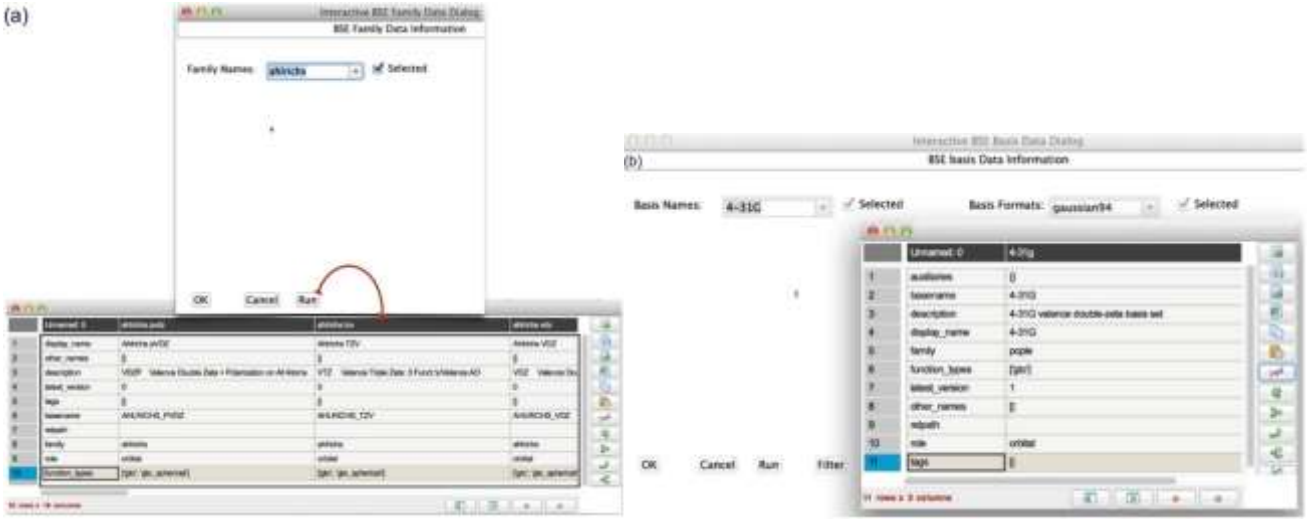

Figure 3 – (a) A single query in the BSE family data, and (b) A double query in the BSE basis data

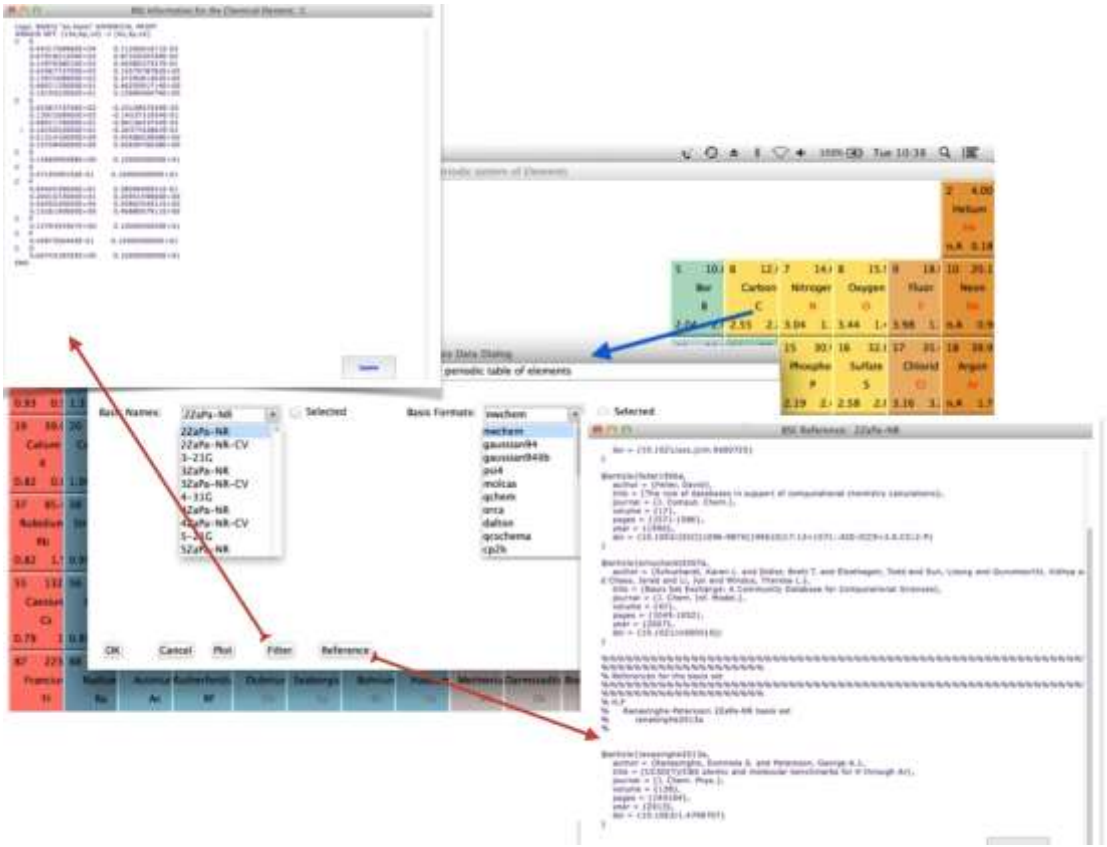

Figure 4: The dialog form for the element carbon (C) from the periodic table

D. Tabular and Graphical Representation

The information about the basis set can also be shown in tabular format using *pandastable* package and its *Table* and *TableModel* modules from Python. Furthermore, the Plotting View module of *pandastable* can create formatted graphs. Fig. 3(a,b) illustrates the use of a Tabular view of the data.

E. Quantum Mechanics Level Molecular Design Gaming

In Fig. 5, we show the design of quantum mechanics molecular design gaming dialog. This is used to (randomly) pick up elements from the periodic table to form a molecule, which then can be treated at the quantum mechanics using the HartreeFock self-consistent field theory to calculate the minimum ground state energy, and other properties (such as coordinates, charges, and dipole). The winner is the one that designed the molecule with the smallest energy value.

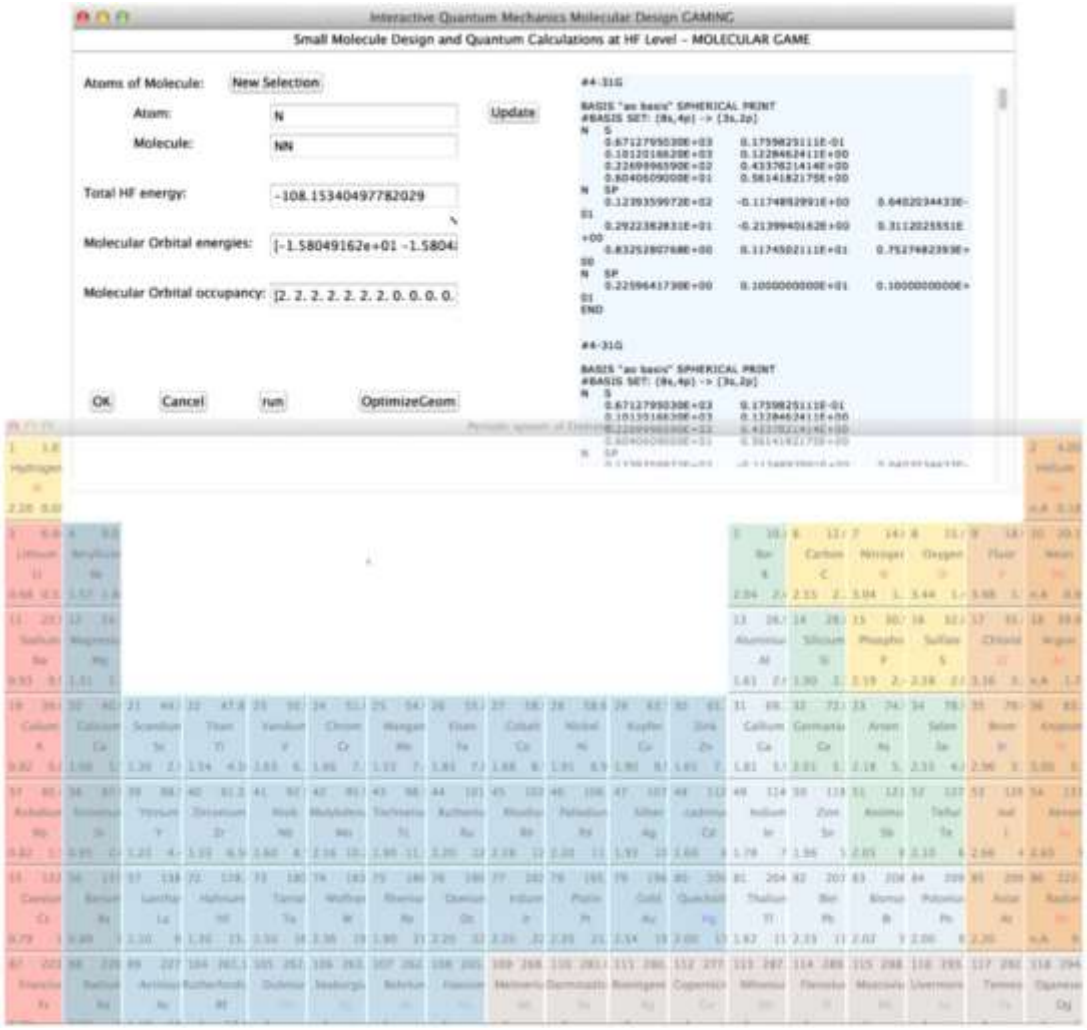

Figure 5: The molecular gaming design at quantum mechanics level

IV.RESULTS WITH ILLUSTRATIVE EXAMPLES

A. Quantum Gaming

This example illustrates the visualization of different types of orbitals for the atom of Carbon (C) using a 3-21G basis set. By clicking on the button *Filter*, after checking the *Selected* checkbox, the information will appear in a new window, as presented in Fig. 6 in the *nwchem* format. According to the information shown in Fig. 6, there are six s-Gaussian types of orbitals that are split into a combination of three s-Gaussian types of orbitals, giving 1s-type of atomic orbital:

$$\emptyset^{(1s)}(r) = \sum_{i=1}^{n} c_i \left(\frac{2\alpha_i}{\pi}\right)^{3/4} e^{-\alpha_i r^2}$$

where n=3 and the vectors of coefficients and exponents are given as

$$\mathbf{c} = (0.06176690738, 0.3587940429, 0.7007130837)$$

$$\boldsymbol{\alpha} = (172.256, 25.9109, 5.53335)$$

When the three sp-Gaussian types of orbitals are split into two 1s(inner)-Gaussian type orbitals (2s-type of atomic orbitals) and two p(inner)-Gaussian type orbitals (2p-type of atomic orbitals), the 2s-type of atomic orbitals with n=2 and the coefficients and exponents become

$$\mathbf{c} = (-0.3958951621, 1.215834356)$$

$$\boldsymbol{\alpha} = (3.66498, 0.770545)$$

The 2p-artomic orbital of Gaussian-type is

$$\emptyset^{(2p)}(r) = \sum_{i=1}^{n} c_i \left(\frac{128{\alpha_i}^5}{\pi^3}\right)^{1/4} x e^{-\alpha_i r^2}$$

where n=2 and the vectors of coefficients and exponents are given as

$$\mathbf{c} = (0.2364599466, 0.8606188057)$$

$$\boldsymbol{\alpha} = (3.66498, 0.770545)$$

The outer shells for both 2s-type and 2p-type atomic orbitals with n=1 and the coefficient and exponent given as

$$\mathbf{c} = (1.00000)$$

$$\boldsymbol{\alpha} = (0.195857)$$

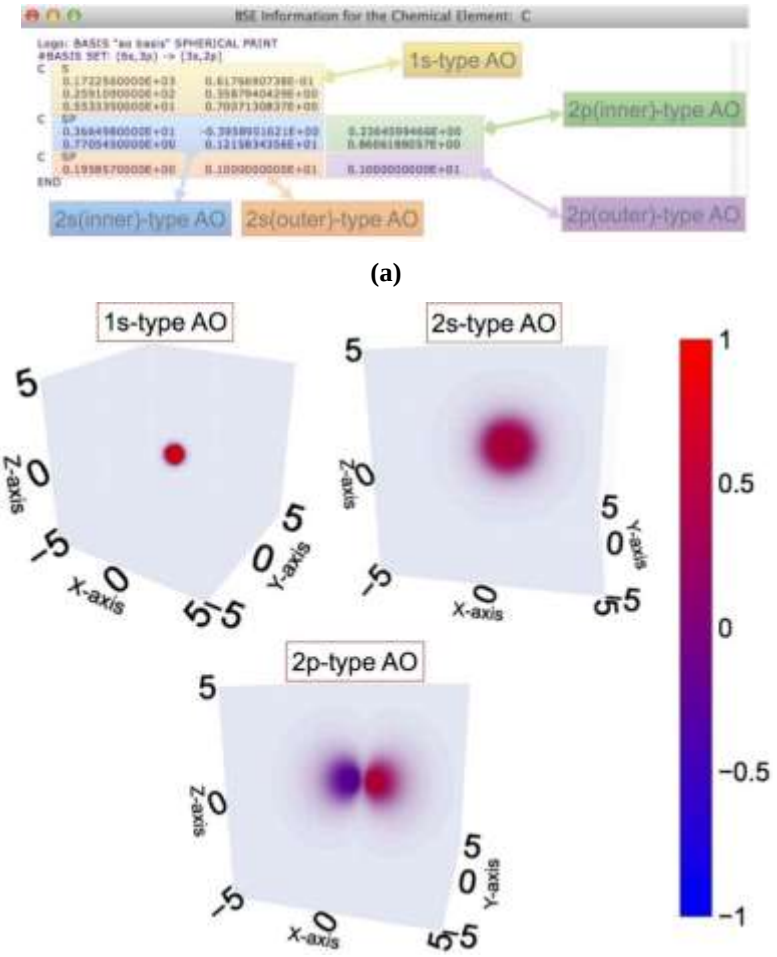

Figure 6: (a) The information about the C chemical element and the basis set 3-21G in the *nwchem* format. (b) The volumetric density plots of $\emptyset^{(1s)}(x,y,z)$, $\emptyset^{(2s)}(x,y,z) = a\emptyset^{(2s)}_{inner}(x,y,z) + b\emptyset^{(2s)}_{outer}(x,y,z)$ for a=b=1, and $\emptyset^{(2p)}(x,y,z) = a\emptyset^{(2p)}_{inner}(x,y,z) + b\emptyset^{(2p)}_{outer}(x,y,z)$ for a=b=1 using 3-21G basis set

The button *Plot* contains the functions for plotting the atomic orbitals as volumetric density data.

B. Virtual Screening

With IPySCF, the optimization and thermodynamic properties of an entire database can be calculated, as depicted in Fig. 7. Different input file formats can be used, such as XYZ, MOL, MOL2, and PDB formats. The IPySCF can use all basis sets provided by the BSE database in different formats (Fig. 7). The three-dimensional molecular structures can be optimized using low or high-cost quantum mechanics calculations using different levels.

In general, the database of molecules can be updated using new molecules designed using a modified version of MolView software, as presented in Fig. 8. In Fig. 9, we listed the thermodynamic properties of ten compounds calculated using quantum mechanics at the Hartree-Fock level. In the given list, the unit of energy is Hartree (Eh) where the environmental conditions were 1 atm (for the pressure) and 298.15 K (for the temperature).

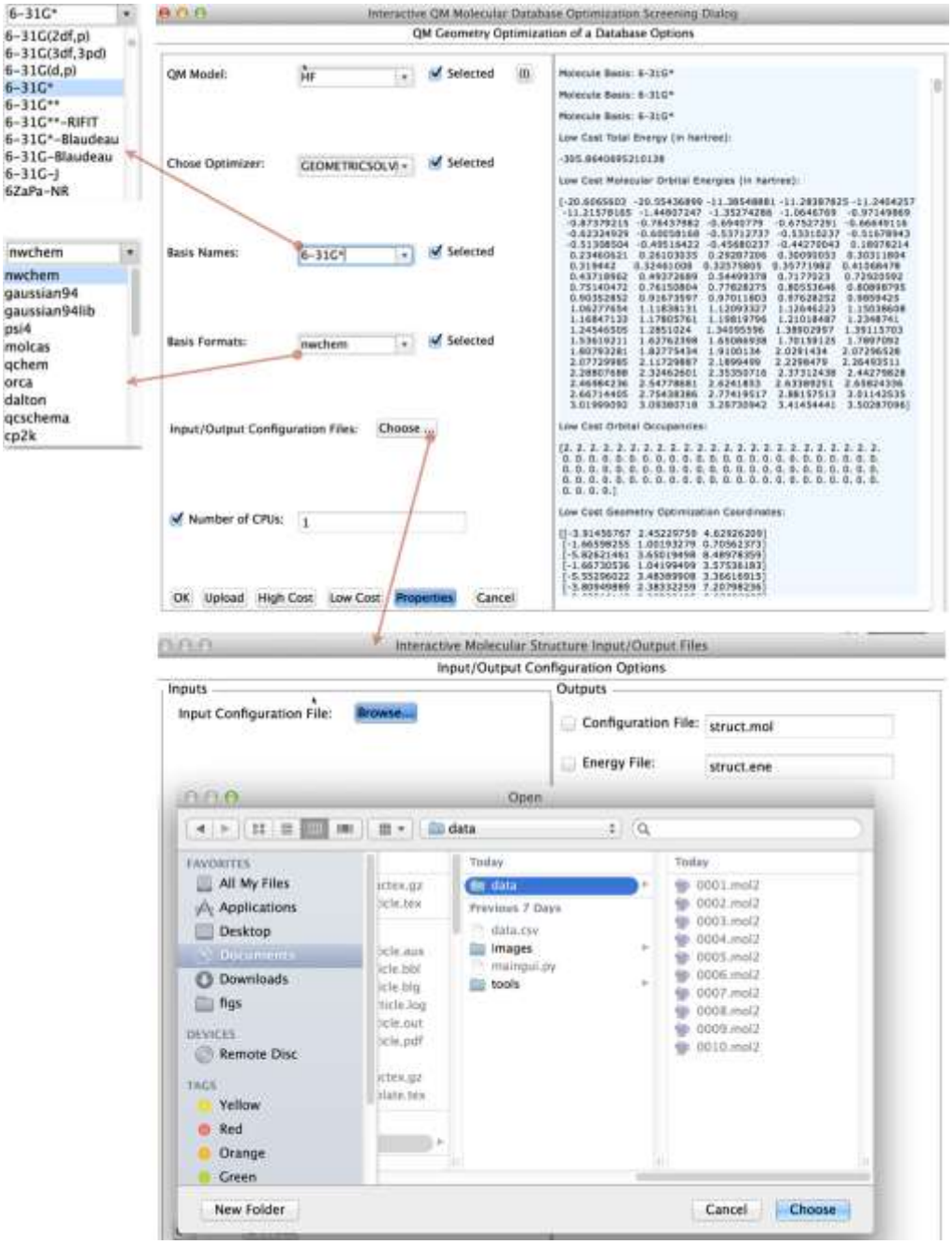

Figure 7: Virtual screening of a database for calculating thermodynamic properties using IPySCF

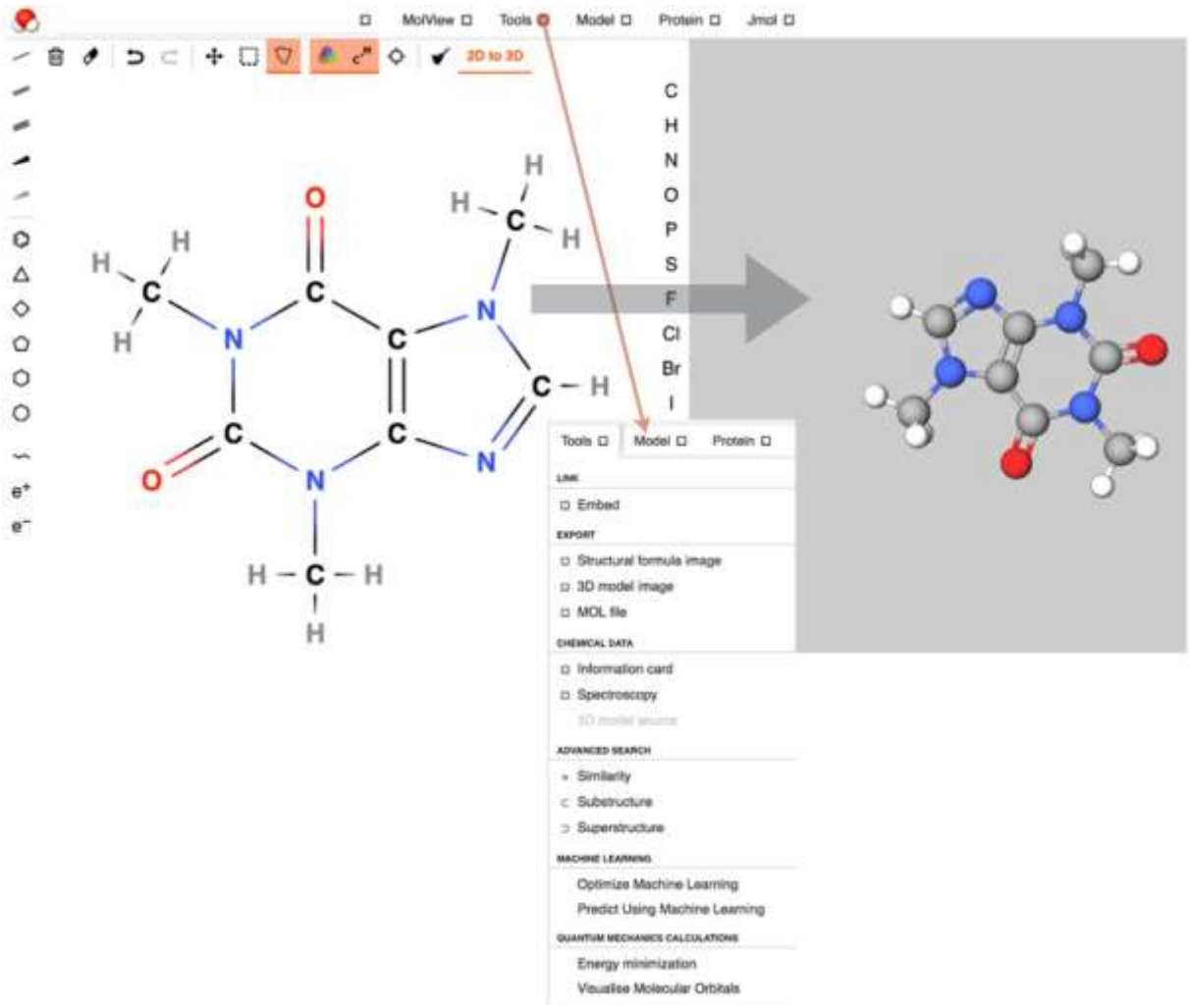

Figure 8: Design and optimization of the two and three-dimensional structure of a molecule

V.CONCLUSIONS AND FUTURE WORKS

This software serves as a crucial interface to query molecular data from the BSE database (Pritchard et al., 2019). It allows users to prepare basis sets in various output formats, including NWCHEM, GAUSSIAN94, DALTON, QCHEM, and JSON, ensuring compatibility with quantum mechanics simulation tools, particularly the PySCF package. The program effectively visualizes atomic orbitals (s-, p-, d-, and f-types) utilizing the *graph_objects* module from *Plotly*, and it can calculate one-center integrals.

It also serves as an excellent educational resource, demonstrating the shapes of atomic orbitals for different elements on the periodic table. Notable contributions include the development of quantum mechanics molecular gaming, the visualization of atomic and molecular orbitals, geometry optimization, a graphical interface for the basis set exchange database, and the innovative design and property calculations for new molecules.

In the current version, we presented an interactive graphical user interface designed in Python for basis set exchange database and quantum mechanics simulations using the PySCF package. Software features included visualization of atomic and molecular orbitals, geometry optimization, graphical interface to basis set exchange database, quantum mechanics properties, quantum gaming, and new molecule design and property calculations. In future versions, we will include interfaces to other packages, such as DALTON, and explore using enhanced computer architectures, such as graphical processing units (GPUs).

Compound	1	2	3	4	5	6	7	8	9	10
name	methyl propanoate	1,3-dichloro-benzene	methanol	2-chloro-phenol	but-1-ene	2-chloro-propane	1,1,1,2,2,2-hexa-chloro-ethane	1,1,2-trichloro-ethane	1,2,3,4,5-penta-chloro-6-nitro-benzene	4-methyl-pyridine
T(K)	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15	298.15
E_0(Eh)	-305.864	-1148.495	-115.032	-764.448	-156.102	-577.166	-2832.537	-1455.910	-2728.544	-285.730
E_{elec}(Eh)	-305.864	-1148.495	-115.032	-764.448	-156.102	-577.166	-2832.537	-1455.910	-2728.544	-285.730
H_{elec}(Eh)	-305.864	-1148.495	-115.032	-764.448	-156.102	-577.166	-2832.537	-1455.910	-2728.544	-285.730
S_{trans}(Eh/K)	6.27E-05	6.51E-05	5.79E-05	6.45E-05	6.05E-05	6.21E-05	6.74E-05	6.47E-05	6.84E-05	6.30E-05
$C_{v,trans}$(Eh/K)	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06
$C_{p,trans}$(Eh/K)	7.92E-06	7.92E-06	7.92E-06	7.92E-06	7.92E-06	7.92E-06	7.92E-06	7.92E-06	7.92E-06	7.92E-06
E_{trans}(Eh)	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03
H_{trans}(Eh)	2.36E-03	2.36E-03	2.36E-03	2.36E-03	2.36E-03	2.36E-03	2.36E-03	2.36E-03	2.36E-03	2.36E-03
sym_{number}	1	1	1	1	1	1	1	1	1	1
S_{rot}(Eh/K)	4.24E-05	4.73E-05	3.02E-05	4.57E-05	3.87E-05	4.05E-05	4.96E-05	4.51E-05	5.33E-05	4.28E-05
$C_{v,rot}$(Eh/K)	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06
$C_{p,rot}$(Eh/K)	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06	4.75E-06
E_{rot}(Eh)	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03
H_{rot}(Eh)	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03	1.42E-03
ZPE(Eh)	1.27E-01	8.68E-02	5.50E-02	1.02E-01	1.16E-01	1.01E-01	1.96E-02	5.23E-02	5.86E-02	1.24E-01
S_{vib}(Eh/K)	1.84E-05	1.73E-05	7.69E-07	1.54E-05	9.79E-06	8.72E-06	3.45E-05	1.44E-05	4.71E-05	1.13E-05
$C_{v,vib}$(Eh/K)	2.51E-05	2.66E-05	2.62E-06	2.66E-05	1.55E-05	1.61E-05	3.77E-05	1.78E-05	5.41E-05	2.19E-05
$C_{p,vib}$(Eh/K)	2.51E-05	2.66E-05	2.62E-06	2.66E-05	1.55E-05	1.61E-05	3.77E-05	1.78E-05	5.41E-05	2.19E-05
E_{vib}(Eh)	1.30E-01	9.01E-02	5.52E-02	1.05E-01	1.18E-01	1.03E-01	2.56E-02	5.49E-02	6.65E-02	1.26E-01
H_{vib}(Eh)	1.30E-01	9.01E-02	5.52E-02	1.05E-01	1.18E-01	1.03E-01	2.56E-02	5.49E-02	6.65E-02	1.26E-01
G_{elec}(Eh)	-305.864	-1148.495	-115.032	-764.448	-156.102	-577.166	-2832.537	-1455.910	-2728.544	-285.730
G_{trans}(Eh)	-1.63E-02	-1.71E-02	-1.49E-02	-1.69E-02	-1.57E-02	-1.62E-02	-1.77E-02	-1.69E-02	-1.80E-02	-1.64E-02
G_{rot}(Eh)	-1.12E-02	-1.27E-02	-7.60E-03	-1.22E-02	-1.01E-02	-1.07E-02	-1.34E-02	-1.20E-02	-1.45E-02	-1.14E-02
G_{vib}(Eh)	1.25E-01	8.50E-02	5.50E-02	1.00E-01	1.15E-01	1.00E-01	1.53E-02	5.05E-02	5.25E-02	1.23E-01
S_{tot}(Eh/K)	1.24E-04	1.30E-04	8.89E-05	1.26E-04	1.09E-04	1.11E-04	1.51E-04	1.24E-04	1.69E-04	1.17E-04
$C_{v,tot}$(Eh/K)	3.46E-05	3.61E-05	1.21E-05	3.61E-05	2.50E-05	2.56E-05	4.72E-05	2.73E-05	6.36E-05	3.14E-05
$C_{p,tot}$(Eh/K)	3.78E-05	3.92E-05	1.53E-05	3.93E-05	2.82E-05	2.87E-05	5.04E-05	3.05E-05	6.67E-05	3.45E-05
$E_{0K)}$(Eh)	-305.737	-1148.409	-114.977	-764.346	-155.986	-577.064	-2832.517	-1455.858	-2728.486	-285.606
E_{tot}(Eh)	-305.731	-1148.402	-114.974	-764.340	-155.981	-577.060	-2832.508	-1455.852	-2728.475	-285.601
H_{tot}(Eh)	-305.730	-1148.401	-114.973	-764.340	-155.981	-577.059	-2832.507	-1455.851	-2728.474	-285.600
G_{tot}(Eh)	-305.767	-1148.440	-115.000	-764.377	-156.013	-577.092	-2832.552	-1455.888	-2728.524	-285.635

Figure 9: The thermodynamic properties of ten compounds calculated using quantum mechanics Hartree-Fock method. The units of energy are Hartree (Eh)

ACKNOWLEDGEMENTS

This study was also supported by Izmir Katip Celebi University Scientific Research Council Agency as project number 2024-TDR-FEBE-0024 for Safa Sadaghiyanfam's doctoral thesis studies.

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