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Examining some mechanical and physical properties of gold

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Abstract: This article utilizes computational software to explore the characteristics of a gold lattice structured in a Face-Centered Cubic (FCC) arrangement. The investigation reveals a heat of formation for gold metal, calculated at 475.2972 kcal/mol, elucidating the energy required for the formation of one mole of gold from its constituent atoms. Infrared (IR) spectroscopy findings are also discussed, with green arrows indicating the normal modes of vibration for gold atoms within the FCC lattice at specific wavelengths. These arrows provide visual representations of the oscillation directions during each vibrational mode when exposed to infrared light. Furthermore, the article examines electronic properties, highlighting the HOMO and LUMO energy levels calculated at -11.61 eV and -7.94 eV, respectively. These levels denote the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), with negative signs indicating bonding orbitals that contribute to material stability. The energy difference of 3.67 eV between HOMO and LUMO influences various properties of gold, such as its electrical conductivity and band gap.

Keywords: Gold, HOMO-LUMO, mechanical properties

Introduction

The direction of oscillation and vibration of gold atoms is a measure to measure the hardness and strength of materials. [1] The greater the direction of oscillation and vibration of the gold atoms of a material, the more tension is needed to change the shape of a certain amount of it. In gold nanoparticles, the atoms on the surface of the nanoparticle are more tightly packed together and stronger bonds are created between them. This makes gold more resistant to deformation and require more force to bend or stretch.[2]

In addition, atomic defects on the surface of gold nanoparticles are less than bulk gold. Atomic defects are weak points in the crystal structure of a material that can initiate cracks and fractures. The lack of atomic defects in gold increases their structural stability and contributes to their greater resistance to deformation.

Increasing the direction of oscillation and vibration of gold atoms in gold nanoparticles creates potential applications in various fields, including:

• Strengthening materials: Gold can be used to strengthen materials such as plastics, ceramics and metals.

• Nanocomposites: gold can be used to make nanocomposites with new mechanical and functional properties.

• Nano devices: gold can be used to make micro and nano electromechanical nano devices.

No single simulation is definitively best for calculating the direction of oscillation and vibration of gold atoms of gold.[3] Choosing the best simulation method depends on several factors, including:

• Accuracy required: If you need atomic-level accuracy, DFT may be the best choice. However, DFT can be computationally expensive and may not be suitable for simulating large systems.

• Computational speed: MD is generally faster than DFT, so it may be a better choice for simulating large systems or studying dynamical phenomena.

• Type of phenomenon studied: MD may be a better choice if you are interested in studying the plastic deformation of gold nanoparticles. However, if you are interested in studying the structural stability of gold nanoparticles, MC may be a better choice.[4,5]

• Experience and expertise of the user: The choice of simulation method also depends on the experience and expertise of the user. Some methods are more complicated to use and interpret the results than others.

Here is a summary of the advantages and disadvantages of each simulation method for calculating the direction of oscillation and vibration of the gold atoms of gold nanoparticles (Table 1)

Table 1 the advantages and disadvantages of each simulation method

Simulation Method	Advantages	Disadvantages
DFT	* High accuracy at the atomic level * Suitable for studying electronic structure and chemical bonds	*Computationally expensive* May not be suitable for simulating large systems
MD	* High speed * Suitable for studying dynamic phenomena * The ability to observe the shape change of nanoparticles when stress is applied	* Lower accuracy compared to DFT * May not be suitable for studying some static phenomena
MC	* High speed * Suitable for studying thermodynamic and statistical properties * Ability to study atomic configurations with low probability	* Lower accuracy compared to DFT * May not be suitable for studying some dynamical phenomena

Scigress is a comprehensive platform for scientific simulation that uses a set of different simulation methods to study various phenomena in different scientific fields, including physics, chemistry, engineering, and life sciences. Scigress is not specifically designed to simulate gold nanoparticles, but It can be used to perform various simulations in this field using the following methods:

• Molecular Dynamics (MD): Scigress includes various MD engines that can be used to simulate the motion of atoms and molecules in gold nanoparticles at the atomic and nanometer scale.

• Monte Carlo (MC) methods: Scigress provides tools to perform MC simulations that can be used to study thermodynamic and statistical properties of gold nanoparticles, such as structural stability and atomic defects.

• Density Functional Theory (DFT): Scigress has a relationship with DFT software that can be used to calculate the electronic structure and properties of gold nanoparticles.

In addition to these general simulation methods, Scigress also provides tools to perform specialized simulations in the field of gold nanoparticles. For example, there are tools to study defect diffusion, nanoparticle growth, and interactions of nanoparticles with other molecules.

Scigress

We focus on Scigress for gold nanoparticle simulation. In this section, we will specifically focus on how to use Scigress to simulate gold nanoparticles.

1. Selecting the simulation module:

Scigress has various modules for MD, MC and DFT simulations. For gold nanoparticle simulation, suitable modules are:

• MD module: This module is used to simulate the movement of atoms and molecules in the gold nanoparticle.

• MC module: This module is used to study thermodynamic and statistical properties of gold nanoparticles, such as structural stability and atomic defects.

• DFT module: This module is used to calculate the electronic structure and properties of gold nanoparticles.[6,7]

Choosing the right module depends on the type of simulation you want to do.

2. Model preparation in Scigress:

Scigress provides a graphical user interface (GUI) and a command line interface (CLI) for importing model and simulation settings.

• GUI: The easy-to-use Scigress GUI allows you to visually create and edit gold nanoparticle models and simulation conditions.

• CLI: The Scigress command line interface offers more power and flexibility, allowing you to perform more complex simulations using text commands.

3. Running the simulation in Scigress:

After preparing the model, you can run the simulation using the "Run" button in the GUI or using the run command in the CLI.

Scigress performs the necessary calculations to simulate the behavior of the gold nanoparticle over time.

4. Analysis of the results in Scigress:

Scigress provides various tools for analyzing simulation data, such as plotting, calculating properties, and visualizing gold nanoparticles.

• Graphing: You can use Scigress graphing tools to graph gold nanoparticle properties over time, such as potential energy, direction of oscillation and vibration of gold atoms, and electronic charge distribution.

• Properties calculation: You can use Scigress properties calculation tools to calculate gold nanoparticle numerical properties such as average potential energy, direction of oscillation and vibration of gold atoms and surface area.

• Gold nanoparticle visualization: You can use Scigress visualization tools to visualize gold nanoparticles over time and in different configurations.

Results

The crystal lattice size of gold nanoparticles can vary depending on factors such as synthesis method, nanoparticle size, and shape. In general, gold nanoparticles have a face-centered cubic (FCC) crystal structure, similar to bulk gold. (Fig. 1) The lattice parameter (the distance between adjacent lattice points) for bulk gold is approximately 0.4078 nanometers. However, the lattice parameter of gold nanoparticles may deviate slightly from this value due to factors like surface effects and strain induced by nanoparticle size reduction. For small nanoparticles, the lattice parameter may be slightly larger due to surface relaxation effects.

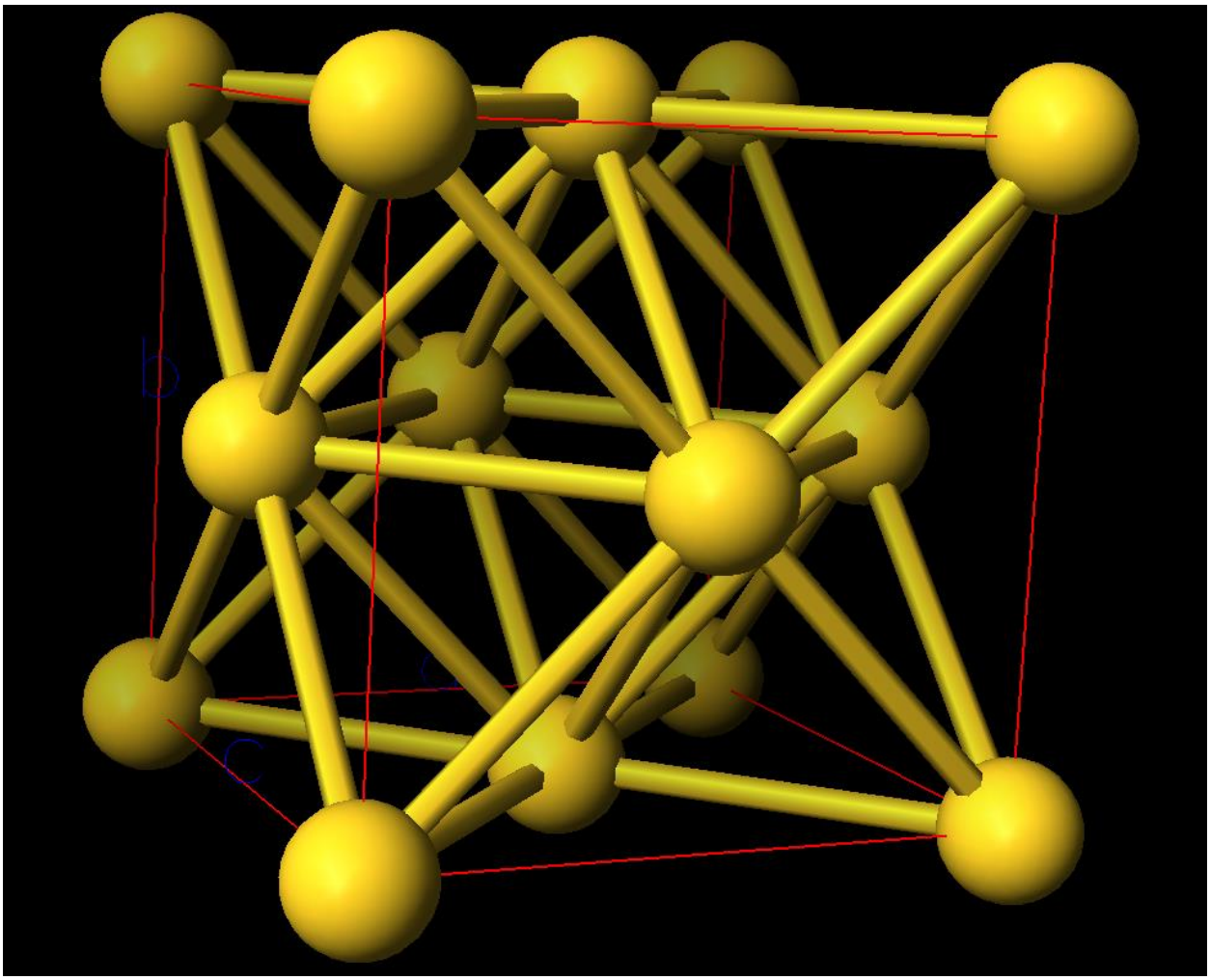

Fig1 Gold FCC

The lattice boundary of gold refers to the boundaries or interfaces between individual crystalline grains in a polycrystalline material. In the context of gold nanoparticles, the lattice boundary typically refers to the region where the crystal lattice of one nanoparticle meets the crystal lattice of another nanoparticle or the substrate material if the nanoparticles are deposited onto a substrate.

These boundaries can have important implications for the properties of the material, as they can influence phenomena such as grain growth, mechanical properties, and electrical conductivity. In the case of gold nanoparticles, the lattice boundaries can affect their optical, electronic, and catalytic properties, making them an important consideration in various applications.

Scigress allows you to define the structure of a unit cell, which is the smallest repeating unit of a crystal lattice. The Fig 2 in the window refers to the crystal system and the fractional coordinates of the atoms in the unit cell.

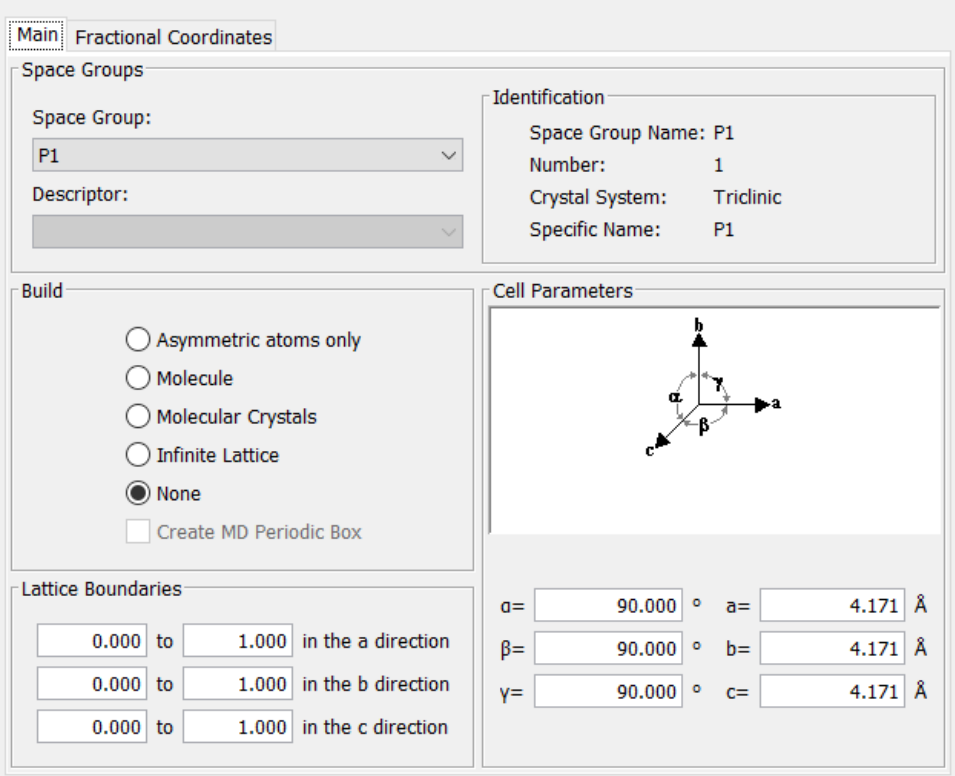

Fig 2 the structure of a unit cell of Gold

Space group: This refers to the symmetry of the crystal lattice. In the image, the space group is P1, which is the triclinic crystal system. This is the least symmetrical crystal system.

Cell parameters: These are the lengths of the edges of the unit cell and the angles between them. In the image, the cell parameters are a = 4.171 Å, b = 4.171 Å, and c = 4.171 Å, and all of the angles are 90 degrees.

Fractional coordinates: These are used to specify the position of an atom in the unit cell relative to the edges of the cell. For example, an atom at (0.5, 0.5, 0.5) would be located at the center of the unit cell. The program allows you to define the positions of the atoms in the unit cell by entering their fractional coordinates. You can then use this information to calculate the properties of the crystal, such as its density and diffraction pattern.

The Fig 3 is a table of atomic positions in a unit cell, likely generated by a crystallographic software program. It shows the fractional coordinates of 15 gold (Au) atoms in a unit cell.

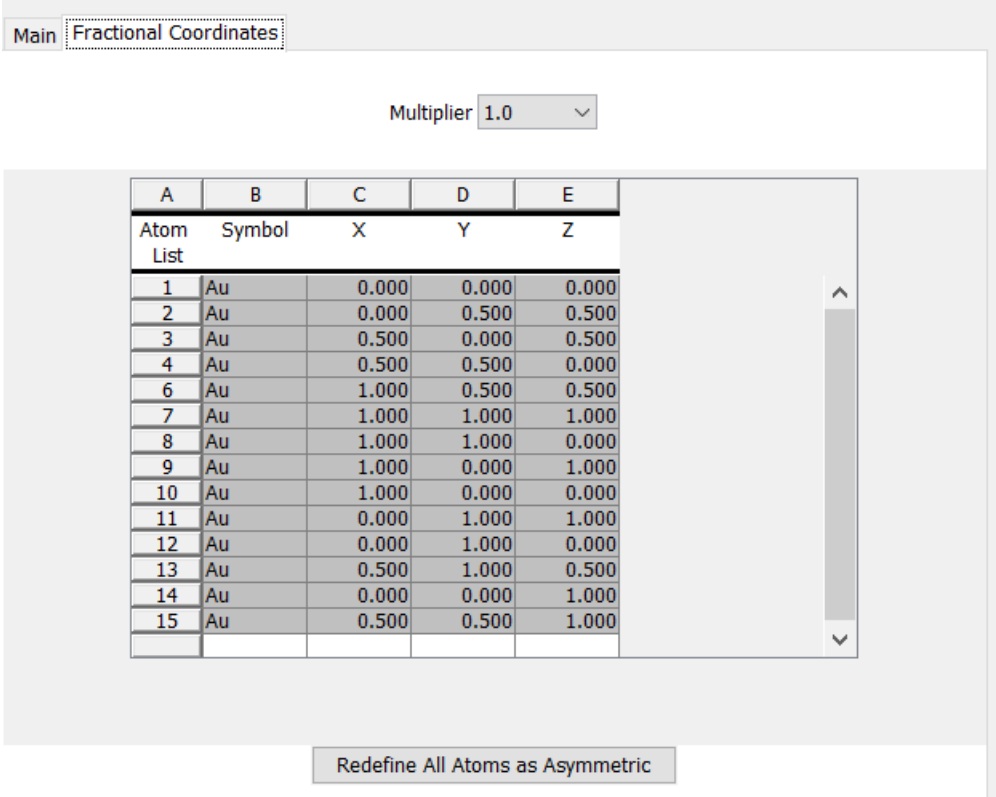

Fig 3 a table of atomic positions in a unit cell

Here's a breakdown of the table: Main Fractional Coordinates: This section specifies the location of each atom relative to the unit cell.

Atom/Symbol: This column identifies the element (Au) and its atomic symbol.

X, Y, Z: These columns contain the fractional coordinates for each atom along the unit cell's a, b, and c axes, respectively. A value of 0.000 indicates the atom is positioned at the origin of the axis, and 1.000 indicates it's positioned at the edge of the unit cell in that direction. Values between 0 and 1 specify a position along the axis relative to the cell edge. For instance, an atom with a Y value of 0.500 would be located halfway along the unit cell's b axis.

Multiplier: This value (1.0 in this case) scales the atomic positions.

List: This section likely refers to a different way of defining atomic positions within the program, but it's not displayed in the image.

Overall, the table describes the arrangement of gold atoms within a unit cell of a crystal structure. This information is useful for understanding the crystal's properties and how the atoms are packed together.

The Fig 4 is a status log energy chart. It shows the progress of a calculation and the energy levels found at each step. The bottom right corner displays the gradient, which is a measure of how quickly the energy changes between steps. A large positive gradient indicates a stable configuration was found, while a large negative gradient suggests the calculation may be approaching an unstable configuration. In essence, the status log energy chart helps a crystallographer monitor the progress of a calculation and assess the stability of the crystal structure being investigated. Final heat of formation = 475.2972 kcal/mol.

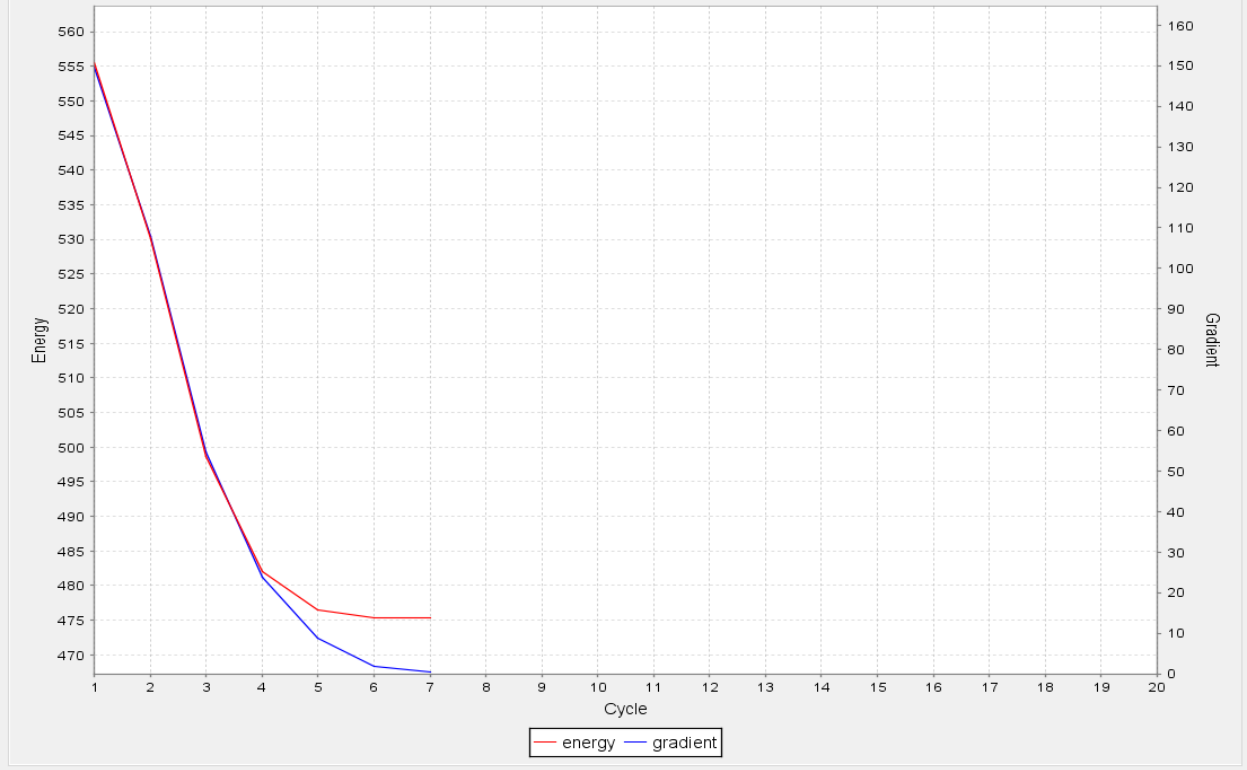

Fig 4 status log energy chart

The Fig 5 is an infrared (IR) spectrum of a sample labeled mp-81 Au. However, since gold (Au) is an element, it does not have functional groups and therefore would not produce an IR spectrum itself.

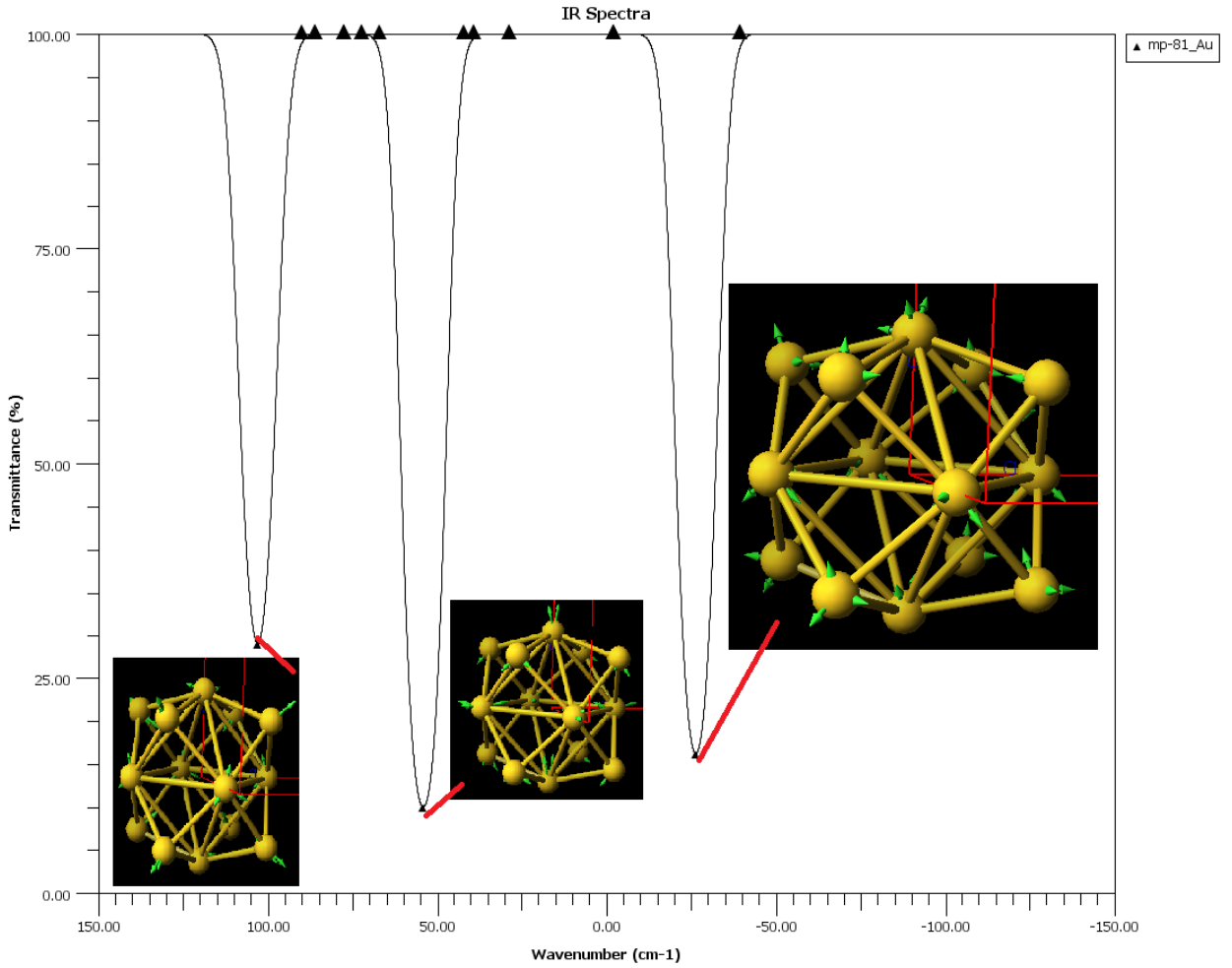

Fig 5 Gold IR spectroscopy

IR spectroscopy is a technique used to identify functional groups within a molecule by analyzing the infrared light the molecule absorbs. The peaks you see in the image correspond to the wavenumbers (cm^-1) of the infrared light absorbed by the sample. The number of peaks and their positions depend on the chemical structure of the molecule being studied, not necessarily Iridium (Ir).

In this case, the IR spectrum likely represents the molecular structure of the material mp-81 Au, which might be a gold compound or a material containing gold along with other elements. Without more context about mp-81 Au, it's impossible to say for sure what the peaks represent.

Here are some additional points to consider:

The spectrum shows four main peaks within the wavenumber range displayed (150 cm-1 to -150 cm-1). It's important to note that IR spectra can sometimes show broad peaks or shoulders that may be difficult to distinguish from the baseline noise. The direction of oscillation of gold atoms is indicated by the green arrow for each wavelength in Fig5.

Fig 6 shows the HOMO and LUMO values of gold. HOMO stands for Highest Occupied Molecular Orbital and LUMO stands for Lowest Unoccupied Molecular Orbital. These values represent the energy levels of the most filled and the least filled electron orbitals in the gold lattice, respectively. Negative signs indicate that these orbitals are bonding orbitals (stable). The energy difference (3.67 eV) between HOMO and LUMO can be related to various properties like conductivity and band gap in gold. The amount of HOMO -11.61 eV and the amount of LUMO -7.94 eV.

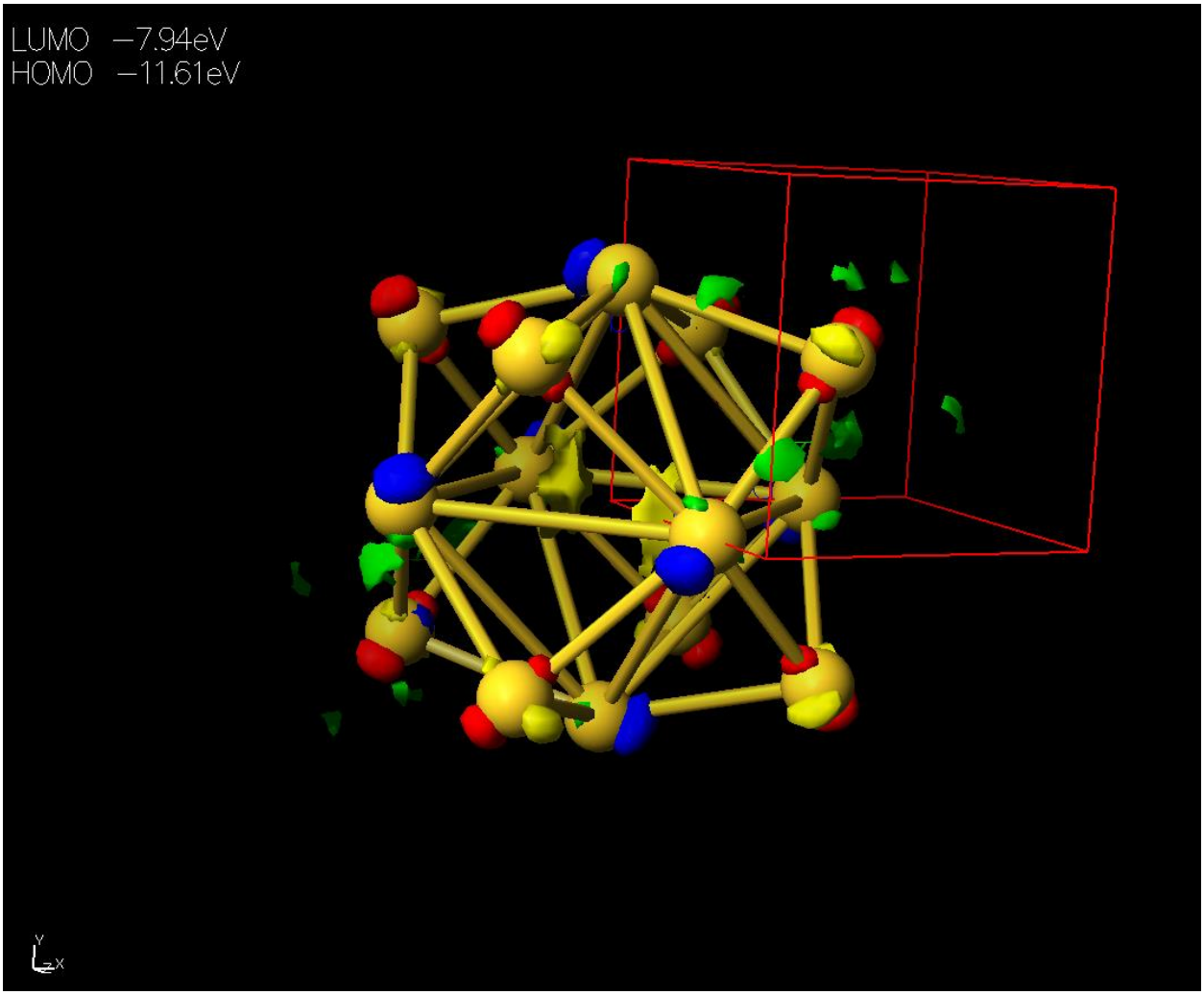

Fig 6 HOMO-LUMO of Gold

Conclusion

In this article, software was used to calculate some characteristics of a gold lattice with a Face-Centered Cubic (FCC) structure. The final heat of formation is reported to be 475.2972 kcal/mol. This value represents the energy required to form one mole of gold metal from its constituent atoms, typically assumed to be in their most stable elemental state.

The article also mentions green arrows associated with specific infrared (IR) wavelengths. These arrows likely depict the normal modes of vibration for the gold atoms within the FCC lattice at those wavelengths. In simpler terms, the arrows visualize the direction of oscillation (movement) that the gold atoms undergo during each vibrational mode when exposed to infrared light of those specific wavelengths.

Finally, the article mentions HOMO and LUMO energy levels, calculated to be -11.61 eV and -7.94 eV, respectively. HOMO stands for Highest Occupied Molecular Orbital and LUMO stands for Lowest Unoccupied Molecular Orbital. These values represent the energy levels of the most filled and least filled electron orbitals in the gold lattice, respectively. The negative signs indicate that these are bonding orbitals, which are energetically favorable and contribute to the stability of the material. The difference in energy between HOMO and LUMO (3.67 eV) can be related to various properties of gold, such as its electrical conductivity and band gap.

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