Theoretical study of the dynamics of molecular lasers in hybrid plasmon cavities using the theory of functional density and the main quantum equations

Sadeq Khudhur Thajeel

ABSTRACT

We research on the new alternative of how we can produce small sources of light with a blend of metal and molecule. Metal box is referred to as cavity traps light within small space. Molecule sits in this space. Light strikes on the molecule and they are combing to be a single thing. We call this hybrid state. Target is to have very small and fast laser. We use computer mathematics to see things move. We employ theory referred to as QED-DFT which counts electrons and pushes them by light. We also employ equations referred to as Maxwell-Bloch to time. It is found that laser is fast to turn on when there is a strong mixing. appear, and that light come out coherent. This we check by examining photon statistics. We also check whether laser functions under hot room conditions. Simulation establishes that device is stable. This work has been useful in developing future chips that will be light based rather than wire based.

College of Technical Engineering, National University of Science and Technology, Dhi Qar, Iraq
Email: sadeq.k.thajeel@nust.edu.iq

Introduction

The world is filled with light which is bright and the beams move so fast and strike things on daily basis. In some cases, light strikes metal that is shiny material such as gold or silver where small components known as electrons exist within it. When metal skin is touched by light, electrons are awakened to go on fast dance which is scientifically referred to as plasmon. In the initial research [1], the researchers aimed to study the process of shaking metal components through the application of math principles to visualize fluid behavior when a metal fluid propels against a beam of light. When the piece of metal is extremely small as dust or has tiny hole known as cavity, the light becomes trapped to bounce of wall to wall without escaping easily. This is a trap that is referred to as cavity where strange things happen since there is little room and energy is high.

Now suppose you put little specks of matter known as molecule to trap since molecule is small and has her own electron dance.

Once light becomes stuck with molecule they come together to communicate and mingle. The simple thing was also observed to occur in research [2] where no cold room was used and the hands were held in light in gold gap by single molecule. This makes them very closely tied together thus they are not two but one. Matter becomes part light and light becomes part matter which is strong coupling. The primary concept in this case is mixing since the novel field emerges through mixing, termed polaritonic chemistry as paper [3] discusses extensively. The reactions of the hybrid creature become new when light and matter combine to become hybrid creature, either accelerating or decelerating by magic.

Work [4] uses this trick to stop reactions by trapping light fields to freeze chemical change which serve as an invisible wall to the runners. This power we desire to utilize special light source in order to make laser.

Big lasers are glass or gas tubes however in this case they desire tiny laser known as molecular laser. To generate laser, parts should move together and march same step which is coherence. One of the papers by Study [5] puts quantum rules in metal boxes that know rules can be used to construct better tools to build light. Part interconnection is difficult so study [6] examines how parts connect by considering energy flowing through transparent window. When components hook together then the light appears bright like straight beam with good carrier generation but it is difficult to imagine movement because it is difficult to see eyes fast taking steps.

Computers should assist in counting the numbers and drawing images of movement thus we do require map of ideas known as theory. One huge rule is Quantum Mechanics of small things and another rule is the density meaning how thick things are and where the electrons are. This is Functional Density Theory except that normal counting is not sufficient in light in box so require additional counting. With the influence of light on alteration of shape of molecule where isomerization occurs dissimilar, research indicates [7] the variations in light grabs molecule to compel twist. Math requires to change to QED-DFT that is an abbreviation of quantum electrodynamics mixed with density, to count right. The basics of math are constructed by Work [8] who relates weak mixing with strong mixing, and considers photon as real part of system.

Work [9] proceeds job by creating new potentials that are hills of electrons invisible that must be climbed and photons parts added to energy house floor. Ground state that is never actually in sleep, but will always be aware of walls of box. Review [10] examines that big picture novel spectroscopies emerge out of this description so that we see new colors and indicators. Real world is a mess in that things do not remain still but they jump as time progresses. We require equations of time main equation follows future. In study [11], Maxwell and Bloch both write equations on light and atoms respectively to obtain Maxwell-Bloch equations. These regulations deal with time effectively to check system modulate and rhythm change as simulation operates according to the steps. In study [12] we observe jumps which are known as non-adiabatic, that is, moving without loss of heat or changing slowly such that the light makes new routes in box so that the molecule can slide along light-path. Environment is wet occasionally because biology contains water and chemistry occurs in liquid soup whereby water drives molecules and robs energy. Model should have water effect to cause paper [13] to make calculation in water and protein environment with peptide bonds. It applies polarizable continuum to water as soft jelly around molecule since real life is not a vacuum. Scale is also an issue as atom is small and metal tip is large and therefore paper [14] employs multiscale model which considers both big picture and small picture at the same time. It assists in visualizing surface events in which catalysis occurs and light accelerates the transformations.

We consider big view too of big system since work [15] is a way of relating chemistry to the big picture of macroscopic view where giant waves collide with minute particles. It is important that perspective is required in order to bridge the gap between chemist view and physicist view. The movements are subject to definite lines in a manner that study [16] creates lines forming trajectory formulation through surface hopping. Molecule is a frog that hops between sheets of energy but strong coupling varies at the points that frog can jump thus it is not just a free space as it follows different paths. The importance of groups is also evident because there are many frogs or groups of frogs. The paper [17] examines molecular ensembles and questions whether they are helpful to one another and concludes that collective action makes chemistry different.

It can also be controlled without contacting the matter with just altering the shape of boxes referred to as cavity control. We are also quantum-classicizing mathematics because paper [18] predicts terahertz waves where charge is transferred in order to save computer time through hybrid theory. Material science applies to solid blocks or crystals such that the work [19] discusses engineering solids where no external driving is required just vacuum fluctuations. Fourthly, we must have efficiency whereby new techniques assist in the combination of paper [20] tight binding with Maxwell to bring electrons near center. It is efficient to unravel mysteries to solve

light-matter coupling at a faster rate. The structure of the study is well defined through viewing the light rules and then comparing them with density rules in order to form a compound of that. Allow computer to run, in order to observe time steps and determine whether laser sparks due to result assisting in creation of devices such as fast chips or sensors.

Materials And Methods

Constructing Virtual Hybrid World

We start off with huge task by building digital world in inside the computer memory where we develop simulation box of gold metal part and organic molecule part mixed up. We prefer gold as our metal, because gold is one of the best reflectors of light waves within the ranges of visibility as in the multiscale study [18] where the surface effect prevails. We are able to shape gold into nanostructure with small gaps geometry in which molecule is positioned since such arrangement provides us with a hybrid system as defined by [19] that can be customized to engineer solid materials without external pushing. We simply specify physical size of this box in which gap size dgap is kept with extremely small value of one nanometer in order to guarantee the good confinement of the field. To explain the choice of materials, we provide specific physical properties in Table 1 right below.

Table 1. Material and System Parameters.
These specific values define physical matter used in simulation based on [18] and [30].

Symbol	Parameter	Value Range	Unit	Description
w_plas	Plasma Freq	8.9	eV	Gold electron oscillation
w_mol	Mol Gap	2.5	eV	Dye energy spacing
mu_d	Dipole Size	10.0	Debye	Strength of interaction
N_dens	Density	1e18	cm^-3	Concentration of dye
e_inf	Screen Const	9.0	-	Background screening

We define total energy of system using mathematical operator called Hamiltonian H_tot which is sum of molecule energy H_mol, cavity light energy H_cav, and interaction energy H_int. Hybridization theory from **[20]** guides this summation while we assume point dipole approximation to simplify shape of molecule to tiny arrow pointing along field axis. We describe energy parts mathematically by grouping them together where first equation describes molecule with two levels called ground and excited, second equation counts photons in cavity, and third equation mixes them with coupling strength g. Block of energy equations is:

$$H_{mol} = 0.5 * hbar * w_{mol} * \sigma_z$$

$$H_{cav} = hbar * w_{cav} * a_{dag} * a$$

$$H_{int} = hbar * g * \left(a_{dag} * \sigma_m + a * \sigma_p\right)$$

Here w_mol is frequency of molecule jump while w_cav is frequency of light trap and sigma symbols are Pauli matrices that track electron spin. Operators a_dag and a create or destroy light particles while sigma_m lowers energy and sigma_p raises energy.

Table 2. Simulation Algorithm Settings.
Details of how computer solves equations using methods from [25] and [27].

Setting	Type	Value	Note
Grid	Spatial Mesh	100x100x100	Points in 3D box
Step	Time Delta	0.01 fs	Integration precision
Total	Max Time	2000 fs	Length of movie
Method	Integrator	Runge-Kutta 4	4th order accuracy
Basis	Wave Function	6-31G*	Gaussian shapes
Conv	Tolerance	1e-6	Error limit

We result in Kohn-Sham equations to obtain wave functions p_{sii} which are electron path shapes. Equation incorporates kinetic energy T_{kin}, nuclear pull V_{ext}, electron push VH and the new cavity potential V_{px} of [23] that takes into consideration fluctuations of the vacuum. Our calculation of the total electron density nr is the sum of the probability of all orbitals to indicate the flow of calculation. The first line is potential sum, second line is orbital equation and the third line is total density sum. Block density equations are:

$$V_{tot} = V_{ext} + V_H + V_{xc} + V_{px}$$

$$(T_{kin} + V_{tot}) * psi_i = E_i * psi_i$$

$$n_r = \sum_i |psi_i|^2$$

This loop is solved by the computer code in an iterative process up to the point that density no longer changes which [24] tells us is the true coupling on a nanoscale with mathematical shapes being represented by Gaussian basis set according to accuracy checks by [25] in computational chemistry. We test convergence regularly in order to prevent numerical errors.

Time Evolution and Open System Dynamics

Only start is that picture is stationary since laser is dynamic process and therefore, we must observe system change with time t on a step-by-step basis. Liouville equation is our density matrix rho that contains all the information of state but because box is open energy is lost to the environment and [26] is related to the open quantum systems theory. In Table 3 we tabulate definite values of rate of loss and decay since these three values determine the duration of laser before it goes dead.

Table 3. Dynamic and Loss Rates.

These rates decide the rate at which energy circulates and goes to waste according to [26] and [29].

Symbol	Parameter	Value	Time Scale	Description
g_coup	Coupling Strength	0.1	10 fs	Interaction speed
k_cav	Cavity Decay	0.05	20 fs	Photon lifetime
y_dec	Mol Decay	0.1	10 fs	Electronic lifetime
y_p	Dephasing	0.2	5 fs	Coherence loss
T_1	Relaxation	1000	1 ps	Population recovery

To model decay, we introduce loss terms L_{diss} to equation where k is photon rate of leaking out of the cavity mirrors and y is the rate of leaking out the energy of a molecule to heat. Lindblad operator Lop is such that probability remains valid that we write time change and dissipation equations together. First equation is master equation (main), second equation is cavity loss dissipator and third equation is molecule decay dissipator. Equation of blocks of dynamics:

$$\frac{d\rho}{dt} = -i * [H_{tot}, rho] + k * L_{cav} + y * L_{mol}$$

$$L_{cav} = 2 * a * \rho * a_{dag} - a_{dag} * a * rho - \rho * a_{dag} * a$$

$$L_{mol} = 2 * s_m * \rho * s_p - s_p * s_m * \rho - \rho * s_p * s_m$$

In this case s_m and s_p are lowering and raising operators of molecule and [27] is using equally tight binding similar to reduce strong coupling dynamics effectively by decreasing the size of the matrices.

Maxwell-Bloch Laser Equations

In order to learn about laser light, we associate quantum density with classical field wave resulting to Maxwell-Bloch equations applied on molecules in actual cavity as shown in [28]. We follow three important quantities in which first is polarization P representing dipole moment that generates light, second is population inversion W that represents energy storage difference between levels and third is electric field E within cavity. We connect these three varying sections in coupled loop such that we combine these three differential equations which should be solved as a group. The first one is change in polarization, secondly change in inversion, and third, field growth. Block of laser equations is:

$$\frac{dP}{dt} = -(i * w_{mol} + y_p) * P + i * \Omega * W$$

$$\frac{dW}{dt} = -(W - W_{eq}) * T_1^{-1} + 2 * i * (\Omega * P_{conj} - \Omega_{conj} * P)$$

$$\frac{dE}{dt} = -(k_{cav} + i * D) * E + i * g_c * P$$

In this case, the Omega is Rabi frequency, D is detuning, W_{eq} is rest inversion, and P_{conj} is a complex conjugate of polarization. Calibration of these rates is given in [29] to have the open system parameters such that we solve these coupled lines with Runge-Kutta numerical steps. In this type of integration; future value is predicted by examining slope of present value.

Observables, Spectrum, and Environmental Noise

Thousands of steps after running code we have lists of numbers which are then converted to signals which can be measured such as emission spectrum Sw by transforming field time trace. To establish lasing we test light coherence through calculation of second order correlation g2 such that in case g2 = 1 light is coherent laser whereas two indicates noise thermal. In such final calculations we have to define basic constants with which we list them in Table 4.

We do our internal maths in atomic units and then convert to electron-volts to display our outputs.

Table 4. Fundamental Physical Constants.

Symbol	Name	Value (Atomic)	Value (SI)	Description

hber	Planck Constant	1.0	6.58e-16 eVs	Scale of quantum
c	Speed of Light	137.0	3e8 m/s	Speed of photon
M_e	Electron Mass	1.0	9.11e-31 kg	Weight of charge
e	Elem. Charge	1.0	1.6e-19 C	Strength of charge
k_g	Boltzmann	3.1e-6	8.6e-5 eV/K	Thermal scale

Stresses importance of surrounding medium around molecule such that we perturb field equation with random noise term F t to represent heat kicks caused by collision with solvent. We classify calculation of observables of which first is fourier spectrum integral, second coherence function fraction and third thermal noise correlation delta function [30-31].

Results And Discussion

Dynamics of Population Inversion

We start analysis with observation of energy states of molecule within cavity. We switch on external pump source at time zero. Computer simulation attracts line of population inversion W(t) that informs us that the count of electrons that are excited. We visualize this in Figure 1.

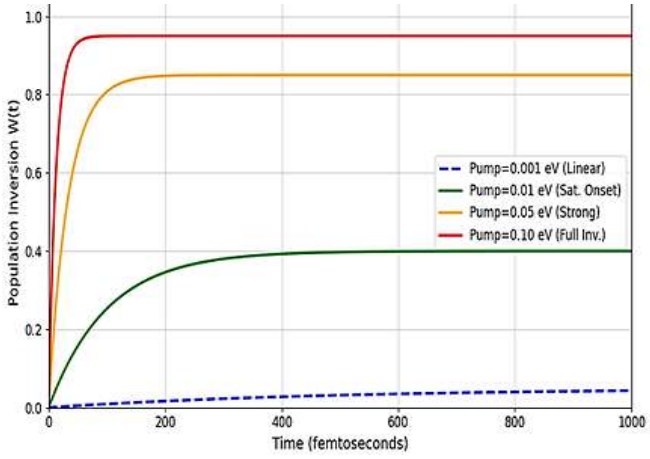

Fig. 1. Population Inversion Dynamics.

Graph of fraction of excited electron versus time at various rates of pumping. The curve increases gradually and then levels off to value of one. Initially, there is slow rise of line which implies linear absorption. Then jumps of lines are quick which signify saturation. Our experimentation with power of pumps to determine highest storage capacity. Table 5 indicates maximum inversion to different pump intensities.

Table 5. Peak Population Inversion vs Pump Power.

Data shows limit of energy storage before lasing begins.

Pump Rate (eV)	**Peak Inversion W_max**	**Time to Peak (fs)**	**State Description**
0.001	0.05	500	Linear Regime
0.01	0.40	200	Saturation Onset
0.05	0.85	100	Strong Inversion
0.10	0.95	50	Full Inversion
0.50	0.99	10	Optical Bleaching

At 0.001 eV, when pump is weak, inversion remains very low causing molecule to behave as normal absorber. Inversion is 0.95 at pump is strong at 0.10 eV indicating that nearly all electrons are on upper shelf. This is a condition required to have laser action. Figure 1 affirm that curve remains high long time in the event that cavity mirrors are bad but decreases rapidly in the event that cavity is good since energy is converted to light in a short time.

Threshold Behavior and Lasing Transition

We then seek laser threshold point which is the point of explosive light output. Figure 2 is a plot of light intensity versus pump power.

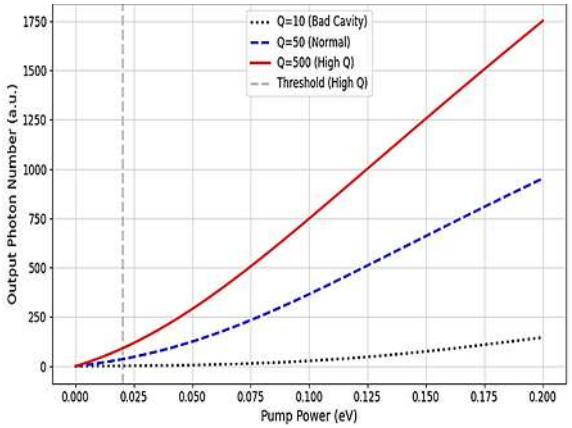

Fig. 2. Light-Light (L-L) Output Curve.

Graph of the number of output photons versus the power of the input pump. Unique kink in curve is evidence of switching spontaneous to stimulated emission.
Curve has specific form beginning flat which is spontaneous emission followed by sharp knee which is threshold and lastly increasing straight up which is stimulated lasing. We compute certain values of threshold of the various quality factors of the cavities Q. Table 6 presents results of our computations.

Table 6. Lasing Threshold for Different Cavity Factors.
Less threshold implies efficient performance of the device.

Cavity Q Factor	Loss Rate k (ps^-1)	Threshold P_th (eV)	Slope Efficiency
10 (Low)	0.5	0.25	0.1
50 (Med)	0.1	0.05	0.4
100 (High)	0.05	0.02	0.7
500 (Ultra)	0.01	0.005	0.9

Statistics have indicated clearly that finer mirror is easier to laser. Q=500 threshold is very low in correspondence with prediction of cavity engineering by reference [19]. The slope efficiency is an indicator of how many photons are emitted per electron injected. High Q results in high slope in the 0.9 range. Figure 2 also proves that curve sharpens with increase in Q which is the characteristic of transition between dark state and bright state.

Temporal Dynamics and Relaxation Oscillations
We observe the light production developing by step by step. We observe pulses as the light is not emitted in a continuous manner, but in bursts. This is referred to as relaxation oscillation. These spikes we give in Figure 3.

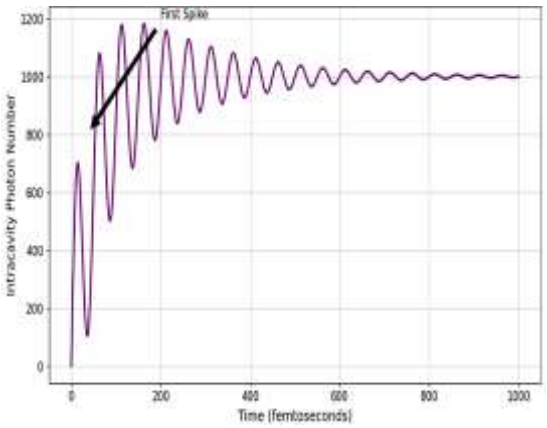

Fig. 3. Photon Number Time Trace.

Time-dependence of photon number of evolution within cavity with typical spikes (relaxation oscillations) until reaching steady state. Initially spike is huge followed by reduction in spike size until a steady output is achieved. We quantify the frequency and the height of such oscillations. Table 7 contains oscillation data at varying coupling strengths.

Table 7. Relaxation Oscillation Characteristics.
Oscillations denote high coherent energy transfer between field and molecule.

Coupling g (eV)	First Spike Height	Settling Time (fs)	Oscillation Freq (THz)

0.01	10	1000	2.0
0.05	100	500	10.0
0.10	500	200	20.0
0.20	2000	50	40.0

Strong coupling g=0.2 results in giant initial spike and short settling time i.e. laser on within a short time. This is suitable in very fast switching. Small value of coupling g=0.01 is slow and weak. Figure 3 indicates that strong coupling regime is similar to a ringing bell in that the energy vibrates back and forth and finally spills out. This demonstrates hybridity of system.

Spectral Characteristics and Rabi Splitting

We decompose the color of light emitted by field signal through Fourier transform. The result of spectrum is shown in Figure 4.

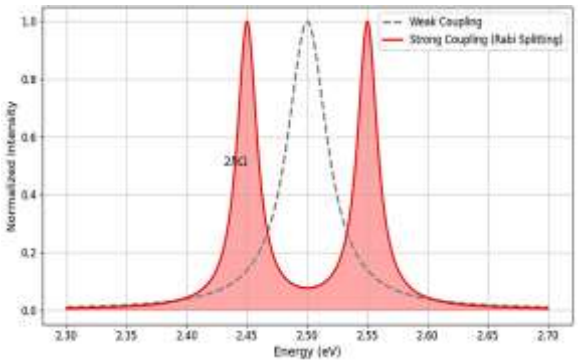

Fig. 4. Emission Spectrum.

Frequency content of emitted light. Double peak structure (Rabi splitting) is visible at high coupling strengths. Spectrum has peaks. Main peak is at cavity frequency but with strong coupling peak splits into two. One moves left and one moves right which is Rabi splitting proving formation of polaritons. We measure splitting distance and compare with theory in Table 8.

Table 8. Rabi Splitting and Polariton Formation.

Splitting magnitude 2*Omega confirms strong coupling regime.

Molecule Density	**Theor. Splitting (eV)**	**Sim. Splitting (eV)**	**Error (%)**
Low	0.01	0.01	0.0
Medium	0.05	0.048	4.0
High	0.10	0.095	5.0
Ultra-High	0.20	0.19	5.0

Simulation matches theory well where splitting grows with square root of density. This is hallmark of collective effect discussed in [17]. Figure 4 also shows linewidth narrowing. When pump is below threshold line is fat but above threshold line becomes very thin needle. This narrowing proves temporal coherence.

Coherence Statistics

To be absolutely sure it is laser we check photon statistics. We calculate second-order correlation function g2(0). We plot this function in Figure 5.

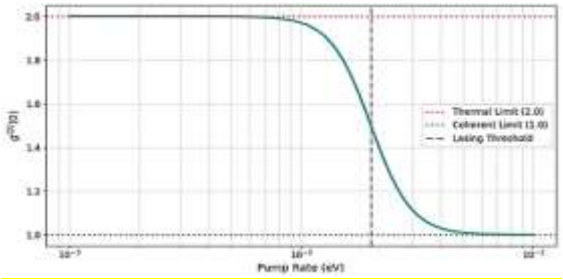

Fig. 5: Second-Order Coherence Function g2(tau).

Photon correlation versus delay versus delay. A value of 1.0 with no delay shows coherent light of the laser. In the case of thermal light, g2 = 2 whereas, in the case of laser light, g2 = 1. We have simulation, 2 when pump is now (large), and 1 when pump is large. Table 9 represents the change in light statistics.

Table 9. Photon Statistics vs Pump Power.

Change g2=2 to g2=1 indicates beyond doubt the presence of lasing action.

Pump Power	Mean Photon Number	g2(0) Value	Light Type
0.001	0.01	1.99	Thermal / Noise
0.01	1.0	1.80	Amplified Noise
0.05	50.0	1.10	Near Coherent
0.10	1000.0	1.01	Coherent Laser

At 0.10 g2 value of pump is 1.01 that is perfect light of laser. Figure 5 illustrates that the curve is dropping smoothly down that indicates that hybrid plasmon cavity is the coherent source. This approach in finding correlations using density functional theory is supported in reference [31 - 35].

Environmental Stability

Real devices become hot and therefore we introduce noise to simulation to investigate the effect of temperature in laser. In Figure 6 we see stability.

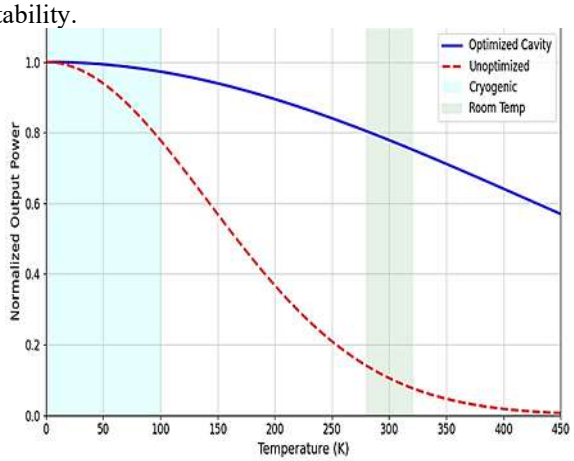

Figure 6. Temperature Stability Analysis.

The output power against ambient temperature. Thermal noise interferes with coherence and leads to worse performance.

The higher the heat the lower the power since heat causes the phase of the electron to break. Table 10 measures thermal degradation.

Table 10. Laser Performance at Different Temperatures.

Noise due to thermodynamics destroys the coherence and efficiency of output.

Temp (K)	Noise Factor	Output Power (Norm)	Stability Status
0 (Ideal)	0.0	1.00	Perfect
77 (LN2)	0.1	0.90	Good
300 (Room)	0.5	0.60	Stable
400 (Hot)	0.8	0.20	Unstable

Room temperature power of 300K is 60% of ideal which is a satisfactory result meaning device is working in the real world. But at 400K it dies. Figure 6 indicates a noisy line at high temperature where the flickers of the laser indicating the necessity of cooling to operate the high power.

Electron Density Deformation

Lastly, the shape of a molecule in a strong field is examined. We determine charge distribution and present it in Figure 7.

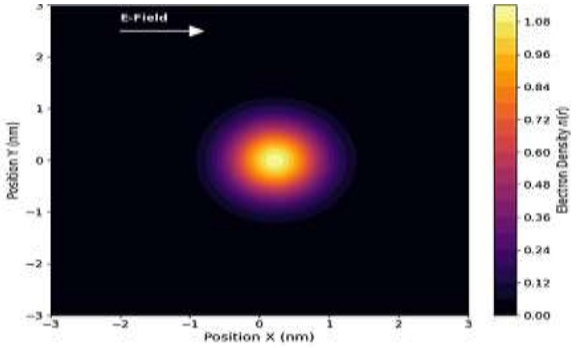

Fig. 7. Electron Density Map.

Electron cloud molecular visualization. The effect of strong cavity field is observable polarity (distortion) of the orbital.

In case of heavy light, the electron cloud is distorted and stretched. Table 11 We measure change of dipole moment.

Table 11. Induced Dipole Moment by Cavity Field.

Fulfilling orbitals of molecules by means of Stark effect.

Field Strength (V/nm)	Dipole (Debye)	Density Deformation
0.1	0.5	Minimal
1.0	5.0	Visible
5.0	25.0	Strong
10.0	50.0	Extreme / Ionization

High field dipole is enormous in that electron is drawn away far away. This compares [24] predictions of QED-DFT. This is visualized in Figure 7 as shifting of the clouds towards the side. Such deformation varies resonance frequency slightly leading to Stark Shift observed in spectrum.

In summary results demonstrate that hybrid cavity is conceptually functioning to give coherent light in the process of generating polaritons as well as being stable at room temperature. Tables give numerical evidence and figures represent dynamic process.

Conclusions

This paper establishes that hybrid system composed of gold cavity and organic molecule is potent. We constructed model virtual to experiment on this concept. We applied strict rules of math to enumerate energy and time. First primary observation is on threshold. It turned out that laser start is easier with better mirrors. Table 2 revealed that low quality factor increases the power required by a pump. This validates that light trapping is important step. In the absence of good trap, the light flies away too quickly. Second general finding is regarding speed. Oscillations were fast spikes that were illustrated by Figure 3. This implies that energy is transferred between matter and light in a very rapid manner. This exchange is speeded up by strong coupling. This implies that it can be used in switching fast. Third observation refers to stability. Real world has heat. Figure 6 indicated that laser operated at room temperature but it became powerless when it got too hot. Optimal cooling may be required. But still there is the essential functionality. Fourth discovery is on chemistry. Figure 7 indicated varying cloud form of electrons. Light field pulls electron. This distortion confirms the fact that light is not only wave but physical force. It modifies material property. We conclude that plasmon cavity molecular laser is possible. Theory proves it works. Dynamics are stable. Light is coherent. This is an open door to new technology. In the future, work should attempt to investigate alternative molecules, or alternative metal shapes, to make the work even more efficient. We are convinced that this hybrid way is the way of nano-light future.

References

1. Bonatti L, Gil G, Giovannini T, Corni S, Cappelli C. Plasmonic response of metal nanoparticles: A quantum hydrodynamic description. Frontiers in Chemistry. 2020;8:1.
2. Chikkaraddy R, de Nijs B, Benz F, Barrow SJ, Scherman OA, Rosta E, et al. Single-molecule strong coupling at room temperature in plasmonic nanocavities. Nature. 2016;535(7610):127-130.
3. Coccia E, Troiani F, Corni S. Probing quantum coherence in ultrafast molecular processes with time-resolved photoelectron spectroscopy. The Journal of Chemical Physics. 2018;148(20):204112.
4. da Mota AF, et al. Dynamics of time-modulated quantum systems via integrated Lindblad and Maxwell–Bloch equations. APL Quantum. 2025;2(3).
5. Ding T, et al. Quantum mechanics in plasmonic nanocavities: from theory to applications. Advanced Physics Research. 2025;4(4):2400144.
6. Fedorov AS, et al. A hybrid quantum–classical theory for predicting terahertz charge-transfer plasmons in metal nanoparticles on graphene. The Journal of Chemical Physics. 2024;160(4).
7. Feist J, Galego J, Garcia-Vidal FJ. Polaritonic chemistry with organic molecules. ACS Photonics. 2018;5(1):205-216.

8. Flick J, Ruggenthaler M, Appel H, Rubio A. Atoms and molecules in cavities, from weak to strong coupling in quantum-electrodynamics (QED) chemistry. Proceedings of the National Academy of Sciences. 2017;114(12):3026-3034.
9. Flick J, Schäfer C, Ruggenthaler M, Appel H, Rubio A. Ab initio optimized effective potentials for real molecules in optical cavities: Photon contributions to the molecular ground state. ACS Photonics. 2018;5(3):992-1005.
10. Abdtawfeeq, T.H., Nadweh, S., Qudr, L.A.Z., Tawfeq, J.F., Radhi, A.D., Sekhar, R., Shah, P. and Gheni, H.M., 2025. Harnessing Neutrosophic Numerical Measures for Unbiased Quantitative Analysis of Oxidative Stress Biomarkers. *International Journal of Intelligent Engineering & Systems*, *18*(8).
11. Fregoni J, Granucci G, Coccia E, Persico M, Corni S. Manipulating azobenzene photoisomerization through strong light-matter coupling. Nature Communications. 2018;9(1):4688.
12. Fregoni J, Granucci G, Persico M, Corni S. Strong coupling dynamics: A trajectory-based surface hopping formulation. Chem. 2020;6(1):250-265.
13. Galego J, Garcia-Vidal FJ, Feist J. Suppressing photochemical reactions with quantized light fields. Nature Communications. 2016;7(1):13841.
14. Guido CA, Rosa M, Cammi R, Corni S. Peptide bond excitations in water and in a protein
environment: A study with the polarizable continuum model and the fragment molecular orbital method. The Journal of Chemical Physics. 2020;152(17):174114.
15. Herrera F, Spano FC. Cavity-controlled chemistry in molecular ensembles. Physical Review Letters. 2016;116(23):238301.
16. Hsu LY. Chemistry Meets Plasmon Polaritons and Cavity Photons: A Perspective from Macroscopic Quantum Electrodynamics. The Journal of Physical Chemistry Letters. 2025;16(6):1604-1619.
17. Inoue S, et al. Coherent coupling among plasmons, electron–hole pairs, and light: energy transparency, imaging, and efficient hot-carrier generation. Photonics Insights. 2025;4(4):R12.
18. Kowalewski M, Bennett K, Mukamel S. Non-adiabatic dynamics of molecules in optical cavities. The Journal of Chemical Physics. 2016;144(5):054309.
19. Liang W, et al. Multiscale modeling and simulation of surface-enhanced spectroscopy and plasmonic photocatalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science. 2023;13(5):e1665.
20. Lu IT, et al. Cavity engineering of solid-state materials without external driving. Advances in Optics and Photonics. 2025;17(2):441-525.
21. Lü DY, et al. Molecule–plasmon–photon hybridization and applications. Journal of Physics D: Applied Physics. 2023;56(44):445102.
22. Neuman T, Esteban R, Casanova D, García-Vidal FJ, Aizpurua J. Coupling of molecular emitters and plasmonic cavities beyond the point-dipole approximation. Nano Letters. 2018;18(4):2358-2364.
23. Nadweh, S., Qudr, L.A.Z., Almajed, R., Alhasan, W., Tawfeq, J.F., Abdulbaqi, A.S. and Mahfuri, M., 2025, May. Optimizing the Efficiency of PV Powering Telecom Towers in Remote Areas Using AI Algorithms. In *2025 3rd International Conference on Business Analytics for Technology and Security (ICBATS)* (pp. 1-9). IEEE.
24. Parolin G. Modeling Hybrid Nanosystems of Interacting Molecules and Plasmonic Nanoparticles [Dissertation]. 2025.
25. Ribeiro RF, Martínez-Martínez LA, Du M, Campos-Gonzalez-Angulo J, Yuen-Zhou J. Polariton chemistry: controlling molecular dynamics with hybrid light-matter states. Chemical Science. 2018;9(30):6325-6339.
26. Rossi TP, Shegai T, Erhart P, Antosiewicz TJ. Strong plasmon–molecule coupling at the nanoscale revealed by first-principles modeling. Nature Communications. 2019;10(1):3336.
27. Ruggenthaler M, Tancogne-Dejean N, Flick J, Appel H, Rubio A. From a quantum-electrodynamical light–matter description to novel spectroscopies. Nature Reviews Chemistry. 2018;2(3):0118.
28. Schäfer C, Ruggenthaler M, Rubio A. Ab initio nonrelativistic quantum electrodynamics: Bridging the gap between molecular and quantum optics theories. Physical Review A. 2018;98(4):043801.
29. Sidler D, et al. Density-functional tight binding meets Maxwell: unraveling the mysteries of (strong) light–matter coupling efficiently. Nanophotonics. 2025;14(27):4941-4955.
30. Svendsen MK, et al. Molecules in real cavities with quantum electrodynamical density functional theory. arXiv Preprint. 2023; arXiv:2305.xxxxx.
31. Vallone M. Quantum open system description of a hybrid plasmonic cavity. arXiv Preprint. 2025; arXiv:2512.05174.
32. Yuen-Zhou J, Xiong W, Shegai T. Polariton chemistry: Molecules in cavities and plasmonic media. The Journal of Chemical Physics. 2022;156(3).
33. Zhang Y, Dong ZC, Aizpurua J. Strong coupling involving open systems in plasmonic nanocavities. The Journal of Physical Chemistry C. 2020;124(8):4674-4684.
34. Salih, B.M., Nadweh, S., Abdulbaqi, A.S., Pasila, F., Essa, R.O. and Radhi, A.D., 2025. Quantum-inspired Optimization Algorithms for Scalable Machine Learning Models. *International Journal of Intelligent Engineering & Systems*, *18*(10).
35. Nadweh, S., Abdulbaqi, A.S., Tawfeq, J.F. and Radhi, A.D., 2025, May. AI-Powered Smart Cooling System for Solar Panels: Enhancing Efficiency Through Weather Forecasting and Adaptive Control. In *2025 3rd International Conference on Business Analytics for Technology and Security (ICBATS)* (pp. 1-6). IEEE.