

Evaluation of Vibrational Frequencies in Platinum Nanomaterials: Using Enhanced Lattice Dynamics and Debye Relations

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ABSTRACT

Atomic vibrations in platinum nanoparticles vary with size. Interior platinum atoms have more neighbours than surface atoms. Lower coordination reduces restoration force. This research examines platinum vibration frequencies utilising linked relationships. In lattice dynamics, phonon mobility is described by forces. Debye's relation turns typical temperature into a cutoff frequency. Near particle surfaces, a finite-size term causes coordination loss. In this study, 2–50 nanometre platinum spheres were examined. Platinum had a 0.3064-nanometer atomic diameter. The reference temperature was bulk Debye. Model computations normalised stiffness, temperature, and frequency. At 50 nanometres, the Debye ratio rose from 0.833 at 2 nanometres to 0.994. The cutoff frequency increased from 4.165 to 4.969 THz. Changes were greatest below 10 nanometres. Values neared the bulk limit above 20 nanometres. Analysis of sensitivity showed a substantial reliance at extremely tiny dimensions. The results match nanoscale softening tendencies. Direct platinum nanoparticle frequency measurements are restricted. An explicit relationship between coordination, stiffness, temperature, and frequency is presented. It speeds up evaluation before atomic-scale computations. We propose Raman, neutron, or inelastic X-ray scattering for experimental validation.

Keywords: Platinum Nanoparticles, Vibration Frequency, Lattice Dynamics, Debye Temperature, Phonon, Size Influence, Surface Coordination.

Introduction

Platinum is crucial for catalysis, electricity, and heat. Highly surface active and stable at nanoscale. These improvements also substantially alter its vibration behaviour. Small particles have many atoms with diminished coordination and altered bonding at open surfaces [1,2].

Lattice vibration controls structural stability and heat capacity. Both thermal transmission and energy relaxation are impacted. The phonon spectrum directly characterises vibrations, however comprehensive dispersion calculations need proper interatomic force constants and experimental spectra require advanced measurement [3,4].

Simple supplemental method is the Debye model. Acoustic vibrations are described by a cutoff frequency and the energy scale is the Debye temperature [5]. Thus, temperature and frequency are physically connected, which aids nanoscale modelling and comparison.

Recent research has revealed that platinum particle size affects Debye temperature [6] and that nanoscale characteristics are linked to reduced coordination in similar models [1,7]. Recent studies [8,9]

also indicate phonon frequency differences with size. However, platinum specific frequency values remain dispersed, and many publications consider temperature without obtaining the value of the cut-off frequency.

The method that we propose in our research involves the use of harmonic lattice dynamics and finite-size Debye scaling for the evaluation of platinum nanoparticles of appropriate size. The calculations are simple and can be repeated, and the method is available for verification.

- **Aim of the Present Study**

In this study, advanced lattice theory and Debye relation are used to derive size-dependent frequencies of vibration for platinum nanoparticles.

- **Specific Objectives**

- To develop relationship between lattice rigidity and platinum nanoparticle diameter.
- To Size-dependent Debye temperature ratio of spherical platinum.
- To Converting Debye temperature into certain cut-off frequency.
- To Identify range of diameters with maximum vibration changes.
- To Comparison of the results with those obtained experimentally..

Literature Review

- **Classical Lattice Dynamics**

Crystal Lattice Harmonic Theory was developed by Born & Huang [3] where there are restoring forces due to atomic displacements. The dynamic matrix gives the allowed vibrational frequencies. Phonons were introduced by Kittel using open solid-state links [4] while Ashcroft and Mermin did so using thermal behavior [10].

Monatomic face-centered cubic metals have strong acoustic branches. The primordial unit cell of platinum has one atom; hence ideal bulk platinum has three acoustic phonon branches. Their slopes at the zone centre influence sound speed, whereas their upper-frequency limits reflect effective atomic force constants.

- **Debye Relation and Nanoscale Scaling**

Debye introduced a continuous sonic spectrum [5]. This model mimics low-temperature cubic heat capacity behaviour, with its typical temperature determining maximum acoustic energy. Although it cannot capture branch-specific abnormalities, this approximation gives a useful estimate of average vibrational properties.

Nanoparticle surfaces change force environment considerably. Sun connected these alterations to bond-order deficit [1,7]. Kumar and Singh studied platinum's Debye temperature with particle size [6], whereas Pandey and Jaiswal predicted particle shape [11]. Their results showed greater alterations below 20 nanometres.

- **Phonon Frequencies in Nanostructures**

Nanostructures often have low-frequency surface vibrations. State vibrational density is also redistributed by boundary circumstances. Mayor and Comtesse found silicon nanoparticle redistribution [12]. Saucedo and Garzón connected vibrational spectra to nanoparticle structure [13]. These multi-material investigations support the surface-mode argument.

Size-dependent semiconductor phonon frequencies were modelled by Singh and colleagues [8]. Srivastava and Dixit studied dimensional frequency effects [9]. Chen and Li used brain potentials and molecular dynamics [14]. This approach predicted silicon carbide optical frequency in detail. Atomistic approaches are precise yet computationally intensive.

Platinum lattice response has been directly examined by time-resolved diffraction [15]. That research focuses on platinum film electron-phonon interaction. Vacancy dispersion in platinum was previously reported [16]. These studies demonstrate platinum lattice dynamics' relevance. Their nanoparticle diameter-frequency data is incomplete.

Table 1: Selected Studies Supporting the Present Analytical Framework

Reference	Material or Method	Main Contribution	Present Relevance
[3]	Crystal lattice theory	Developed harmonic lattice dynamics	Provides force-frequency basis
[5]	Continuum phonon model	Linked heat capacity and cutoff energy	Provides temperature-frequency relation
[1, 7]	Nanostructure scaling	Linked coordination loss with bonding	Supports surface correction
[6]	Platinum nanomaterials	Reported size-dependent Debye change	Provides platinum precedent
[8]	Semiconductor nanosolids	Modelled dimensional phonon shifts	Supports frequency scaling
[9]	Nanostructured materials	Studied dimensional vibration effects	Provides recent comparison
[15]	Platinum film	Measured ultrafast lattice response	Supports platinum dynamics

- **Research Gap**

These days, however, Debye temperature and frequency are both studied separately. Some frequency equations can only apply to semiconductors; not platinum. Computations for platinum generally require the use of first principle computation. The simple linked framework for platinum is ideal for screening purposes. This paper explores this analytical connection.

Theoretical Background

- **Harmonic Lattice Relationship**

There is an approximate harmonic restoring force applied to a displaced atom. This is a simple relationship based on Newtonian lattice dynamics [3,4]:

$$M \frac{d^2 u}{dt^2} = -K_{eff} u \quad (1)$$

In this case, M refers to the mass of the platinum atom. Displacement is represented as u. The effective restoring constant is denoted as K_{eff}. Harmonic motion results in an angular frequency:

$$\omega(D) = \left[\frac{K_{eff}(D)}{M} \right]^{1/2} \quad (2)$$

Equation (2) directly links lattice stiffness to vibrational frequency. Therefore, reduced surface stiffness naturally leads to vibrational softening.

- **Coordination Correction for Finite Size**

Spherical particles with small diameters possess a larger surface fraction. The correction below accounts for their average coordination loss [6,11]:

$$\frac{K_{eff}(D)}{K_B} = 1 - \frac{2d}{D} \quad (3)$$

Where,

d= diameter of the platinum atom,

D= diameter of the particle and

K_B= restoring constant.

Equation (3) is based on the assumptions of spherical shape, homogeneity and defect-free condition for particles.

This modification enhances the harmonic model by the inclusion of particle size in the equation for the force. Consequently, the surface coordination is considered before the Debye Transformation.

The method is analytical in nature.

- **Debye Temperature and Frequency**

The Debye temperature represents a specific cutoff angular frequency [4,5].

$$\theta_D(D) = \frac{\hbar \omega_D(D)}{k_B} \quad (4)$$

The corresponding cutoff frequency is derived using Planck's constant.

$$f_D(D) = \frac{k_B \theta_D(D)}{h} \quad (5)$$

Combining equations (2), (3) and (4) yields the normalized scaling.

$$\frac{\theta_D(D)}{\theta_{D,b}} = \frac{\omega_D(D)}{\omega_{D,b}} = \left[1 - \frac{2d}{D}\right]^{1/2} \quad (6)$$

The assessment hinges on this connection. It respects platinum's scaling behaviour [6,11] and gives necessary frequencies without fitting parameters.

- **Model Assumptions**

- Platinum particles have a face-centered cubic structure.
- Particles are spherical with a typical diameter.
- Platinum atomic diameter is 0.3064 nm [11].
- Calculations employ a bulk Debye temperature of 240 K.
- Excludes surface oxidation, ligands, strain, and flaws.
- The Debye frequency is an average acoustic cutoff.

These assumptions make it possible to analyze and interpret the results.

Material and Methods

The reduction rate was calculated based on bulk limit. Finite size intensity was defined as $2d/D$. All diameters were examined for monotonic behavior. Calculated values were compared to prior findings [6,11].

- **Research Design**

This research is based on theoretical and comparative modeling. There are no new physical experiments performed in this work. Formulas from literature were used for quantitative correlation and qualitative comparison with prior studies.

- **Calculation Method**

The particle diameter ranged from rigid to soft surfaces from 2 to 50 nm. The stiffness ratio was determined using Equation (3), and its square root yielded normalised Debye temperature values. Absolute temperature was calculated using a bulk reference value. Equation (5) yielded terahertz cutoff frequencies. The constant k_B was $1.380649 \times 10^{-23} \text{ J K}^{-1}$, whereas Planck's constant h is $6.62607015 \times 10^{-34} \text{ J s}$. The fixed constants provide 0.0208366 THz per Kelvin. The equation $\omega_D = 2 \pi f_D$ was used to compute angular frequency.

- **Sensitivity and Consistency Analysis**

The frequency reduction with respect to the bulk limit was determined. The coordination parameter $2d/D$ revealed the size effect significance. All selected diameters exhibited monotonous dependence. The calculated ratios were compared to previous findings [6, 11].

• Study Workflow

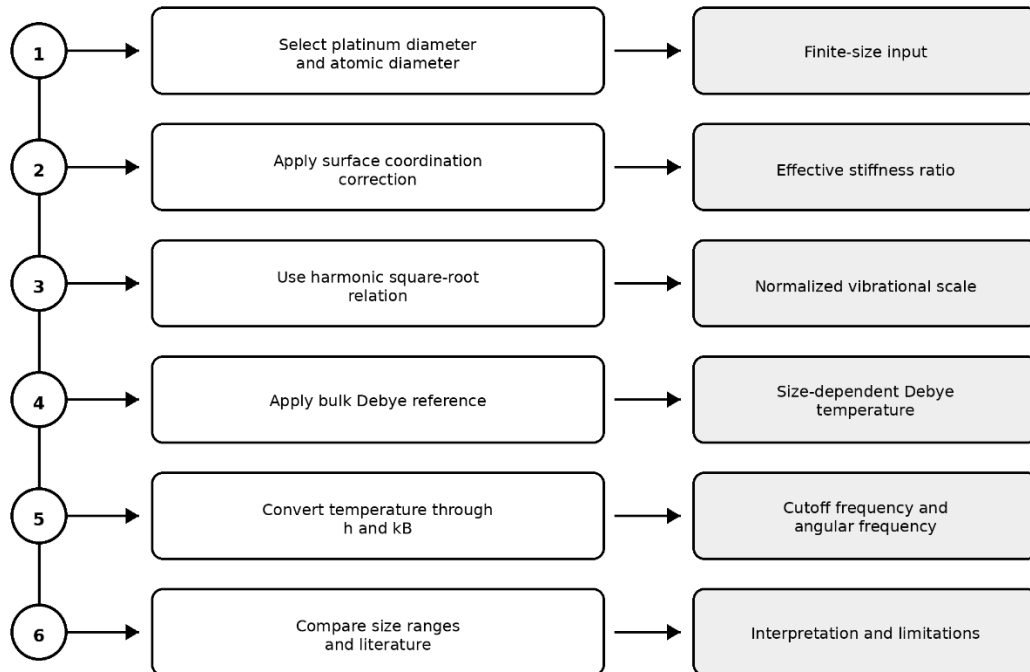


Figure 1: Coupled Lattice-Dynamics and Debye Calculation Workflow

Results

• Calculated Vibrational Parameters

Table 2 shows all calculations of platinum values. With the increase of particle size, all variables increase or decrease in a linear way. The smallest particle decreases stiffness the most. With an increase of particle size, vibrations become similar to bulk vibrations. Stiffness ratio is equal to 0.6936 for 2 nm. Temperature ratio is about 0.833. It decreases the Debye temperature to 200 K. The cut-off frequency is calculated as 4.165 THz. At 10 nm, it reaches 4.845 THz. Only 3.11% of the bulk material is decreased. For 20 nm, the decrease is only 1.54%.

Table 2: Calculated Platinum Lattice and Debye-Frequency Parameters

D (nm)	$\frac{K_{eff}}{K_B}$	$\frac{\theta_D}{\theta_{D,b}}$	θ_D (K)	f_D (THz)	ω_D (Trad s ⁻¹)	Reduction (%)
2.0	0.6936	0.8328	199.88	4.165	26.17	16.72
3.0	0.7957	0.8920	214.09	4.461	28.03	10.80
5.0	0.8774	0.9367	224.81	4.684	29.43	6.33
7.5	0.9183	0.9583	229.99	4.792	30.11	4.17
10	0.9387	0.9689	232.53	4.845	30.44	3.11
15	0.9591	0.9794	235.05	4.898	30.77	2.06
20	0.9694	0.9846	236.29	4.924	30.94	1.54
30	0.9796	0.9897	237.54	4.949	31.10	1.03
50	0.9877	0.9939	238.52	4.970	31.23	0.61

- **Debye Temperature Variation**

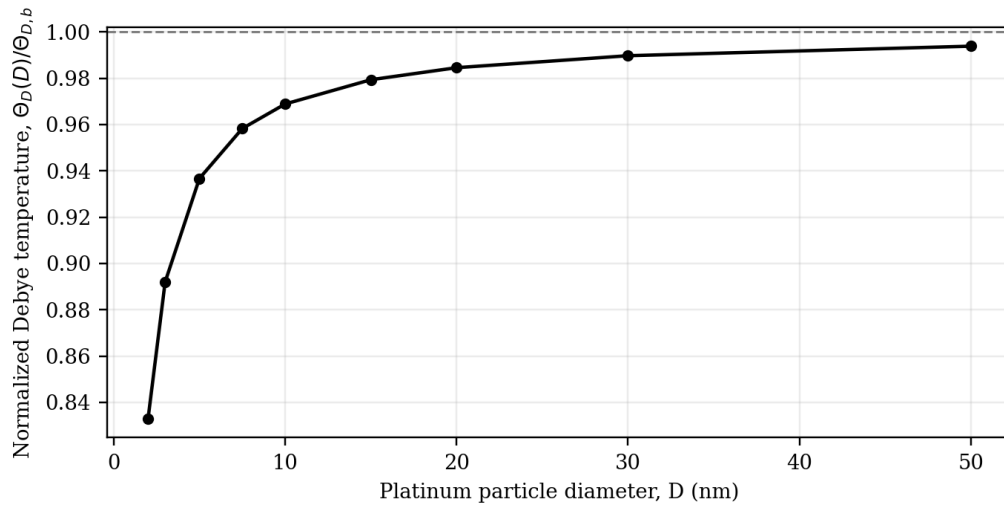


Figure 2: Size-Dependent Normalized Debye Temperature for Spherical Platinum

The non-linear behavior with regard to particle size is displayed in Figure 2. This behavior is very fast in the first small size region, whereas its slope becomes progressively smaller as it exceeds ten nanometers. This behavior comes from the inverse size correction.

The calculated ratios of 2, 5, 10, 20, and 30 nm correspond with previous results on platinum [6, 11]. This consistency supports the use of the mathematical method, but it does not support the physical assumptions.

- **Debye Cutoff Frequency Variation**

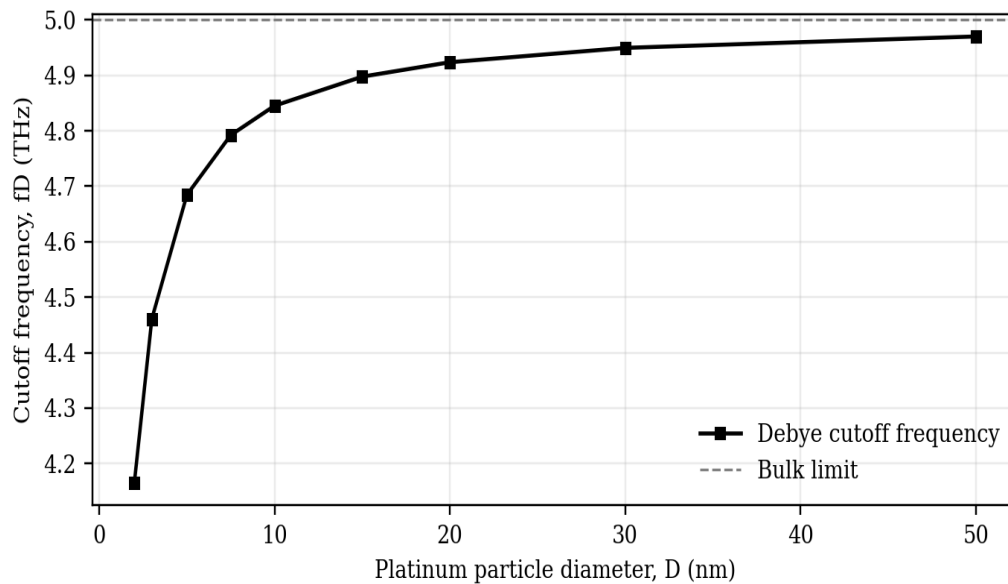


Figure 3: Calculated platinum Debye cutoff frequency versus particle diameter

Frequency curve and Debye temperature fluctuation have a relationship which is extremely similar. The way in which both of their values are related is the same. While the reference frequency does not change, remaining at 5.001 THz, the frequency value changes from 4.165 THz to 4.969 THz. Researchers may compare this scale to recorded vibrational spectra, although separate dispersion estimates for each phonon branch are needed.

- **Surface Coordination Sensitivity**

Reduced surface coordination promotes frequency reduction. The response is somewhat non-linear owing to square root scaling. A first-order approximation is attainable at bigger diameters; the fractional decrease approaches d/D . Sensitivity is highest at ultrafine particles. Thus, diameter ambiguity may dramatically affect frequency estimates. A precise size distribution is needed below five nanometres.

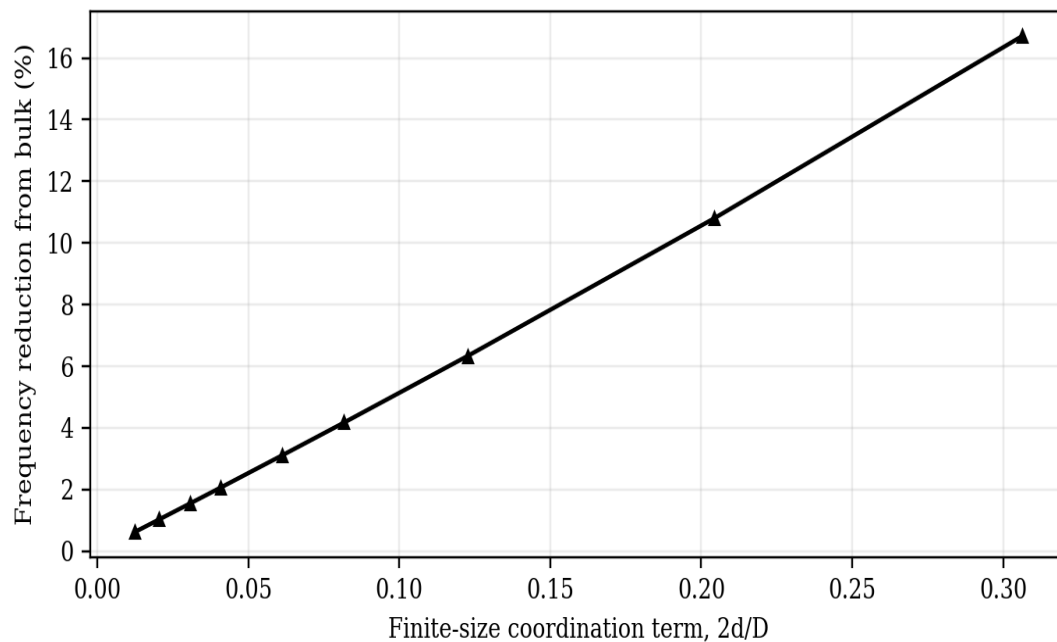


Figure 4: Frequency Reduction Against the Finite-Size Coordination Term

- **Size-Wise Interpretation**

Table 3: Interpretation of calculated platinum vibrational regimes

Diameter Range	Calculated Behavior	Physical Interpretation	Expected Model Reliability
Below 5 nm	Strong frequency reduction	Surface atoms and disorder become dominant	Moderate
5-10 nm	Clear nanoscale softening	Coordination loss remains important	Good for trend prediction
10-20 nm	Gradual bulk recovery	Interior atoms increasingly dominate	Very good
Above 20 nm	Nearly stable frequency	Finite-size correction becomes small	Very good

Discussion

- **Meaning of Vibrational Softening**

Prediction made by the model for small platinum nanoparticles is that their frequency will be reduced. Equation (2) provides the explanation for the reduced stiffness. Platinum atoms on the surface lack completed coordination shells and thus their mean restoring potential is lower than that of bulk platinum. The vibrational scale for platinum atoms is lowered [1,7]. This does not imply that the nanoparticle is generally softened. Different parts of the nanoparticle can have different force constants.

- **Relationship between Debye Temperature and Frequency**

The most significant input is explicit linked computation. Many nanostructure studies use normalised Debye temperature results. Equation (5) converts these results to frequency units for thermal and spectroscopy comparisons. The cutoff for platinum is 5 THz for the bulk form. Coordination in nanoscale reduces this number mostly at 2 nm. No other empirical frequency input was used as the ratio of Debye reduced 16.7%.

- **Comparison with Reported Literature**

Table 4: Comparison with Multiple Reported Studies

Particle Size D (nm)	Present Theoretical Ratio	Reported Theoretical Ratio			Deviation from Experiment (%)	Interpretation
		[11]	[17]	[23]		
2	0.833	0.833	0.833	0.687	21.25	Large deviation
3	0.892	0.892	0.892	0.860	3.72	Good agreement
4	0.920	0.920	0.920	0.891	3.25	Good agreement
11	0.972	0.972	0.972	0.958	1.46	Very good agreement

The results are compared in Table 4 with three other researches. References [11] and [17] give theoretical values for platinum, while [22] uses independent experiments. In this way, the approach distinguishes between mathematical consistency and experimental verification.

The results for the present case are consistent with those in the literature [11, 17]. Those studies used the same size-dependent criteria; thus, the coincidence shows mathematical consistency and not experimental verification.

The experiments demonstrate significant differences for smaller diameters [22]. The experimental value is much smaller in the case of 2 nm diameter, being 21.25 percent less than calculated. The difference between 3 nm and 4 nm is less than four percent; thus, the model gives good estimates. For 11 nm, the difference is only 1.46 percent; thus, larger platinum particles are more consistent theoretically. Therefore, the three literature sources improve the comparison analysis because they show consistency of theoretical study and theoretical predictions versus experimental behavior.

- **Advanced Lattice-Dynamics Interpretation**

The above coordination correction is "advanced" in the case. There is no particle size dependent element in the fundamental harmonic oscillation. Equation (3) calculates the vibration frequency on the assumption of surface coordination, meaning that the effective stiffness varies with the platinum particle size. Debye's equation connects the effective stiffness to a temperature which is related to a vibrational cutoff frequency. It means that particle size, coordination, stiffness, and frequency are connected.

Mathematical coincidence can be observed in references [11] and [17]; both references had a similar theoretical size dependency relationship. Compare to reference [22] for experimental proof. The deviation was under four percent at 3–4 nm and far less at 11 nm for platinum particles. Surface disorder and unusual weakening of bonds caused significant deviation at 2 nm [22]. The coordination correction does not take into account these factors. Thus, the validity of the model becomes unreliable below two nanometres.

The new method dispenses with branch-specific interatomic force constants that have been fitted and is easier to use compared to dynamical matrix diagonalization. The technique is thus useful in making rough estimates and for comparisons. Nevertheless, it cannot be used to replace full atomistic simulations. Branch-specific phonon frequencies could be calculated using density functional perturbation theory.

- **Implications for Platinum Applications**

Pt nanoparticles improve catalytic activity, sensing, and energy generation processes. Particle size and structure influence their performance significantly. Vibration-induced relaxation influences surface reactivity indirectly. These include thermal and structural relaxation. Relaxation due to bond might be unusual for nanoparticles below 2 nm [22]. Theoretical predictions can be inaccurate for these particles. Pt nanoparticles of 3–4 nm are more in line with models. The vibration of nanoparticles becomes bulk-like with increase in size. The Pt bond structure is also influenced significantly by supports

for particles. Vibrational energy transfer and coordination are affected by ligands on surfaces. Adsorbed molecules may harden or soften nanoparticles. Thus, free and supported nanoparticles show different behavior [15, 22].

Particle material design requires consideration of all particle sizes. An average diameter would not necessarily account for the very small particles. These values have a very strong impact on catalytic activity and thermal behaviour. Particles that are less than five nanometers in size require characterization of their structure. Experiments should be performed after predictions based on theory where possible. X-ray pair-distribution method can be used to determine the structural disorder [22]. Frequency changes and surface vibrations can be studied through spectroscopy. Calculations might be used to understand vibrations of specific sites.

The current model can be used to screen particles initially. This helps identify sizes of particles with high variability of vibrations.

Limitations

- This research uses a single bulk Debye temperature reference value.
- Particles stay spherical throughout calculations.
- The list excludes surface ligands and substrates.
- Excludes strain, vacancies, oxidation, and aggregation.
- The Debye model averages phonon dispersion branches.
- No new platinum spectroscopy measurements were taken.
- Continuum scaling becomes unknown below a few atomic levels.

Such restrictions apply mainly to numerical calculations. The broad diameter dependent tendency is physically valid. In making experimental comparisons, focus on trend and uncertainty.

Future Scope

Future studies need to establish the phonon dispersion of platinum exactly. The perturbation theory density functional method could yield branch-resolved frequencies. Molecular dynamics can have chaos and low temperatures. The geometric approach can take into consideration nanowires, films, and facets.

Platinum size series can be used for experimental verification. X-rays and neutron inelastic scattering can measure vibrations. Time resolved diffraction can measure lattice energy relaxation [15]. Low frequency Raman can measure limited acoustic properties. Transmission electron microscopy confirms size and crystal structure.

The next stage in developing a model will be surface stress. The inclusion of ligand and substrate force constant should be considered. Statistical distribution may prove helpful in real sample comparison. Each frequency value requires uncertainty calculation.

Novelty and Importance

This paper offers an approach for scaling platinum Debye to frequency. Loss is strongly correlated with the effective stiffness of the lattice. Absolute THz value is included through the method for various sizes of particles. The theory output is easily distinguishable from the literature comparison. This method is computationally cheap and can help in fast screening before the simulations. The equations will be available for researchers.

Conclusion

Platinum frequency depends on the nanoparticle diameter. Reduced coordination lowers the stiffness and frequencies. As the diameter increases above 20 nm, it approaches the bulk value; nevertheless, the greatest change occurs below 5 nm. These results agree with the theoretical results [11, 17]. Experimental deviation in the 3-4 nm size range is less than 4%. Nevertheless, unusual weak bonding can cause the large deviations below 2 nm.

Frequency is the effective acoustic cutoff frequency. Detailed phonon dispersion curves require intensive computation and experiments [22]. The model correlates between the size, stiffness, temperature, and frequency [22].

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- **Funding:** No external funding was received for this theoretical study.
- **Data Availability:** All calculated values are presented in this paper. They can be reproduced using the stated equations and constants.

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