Quantum–Electrochemical Modeling of Nano-Capacitance Under Electric and Magnetic Fields

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ABSTRACT

Energy storage at the nanoscale is a crucial aspect of next-generation clean energy technologies, including solar energy conversion and electric mobility. In this study, a novel quantum–electrochemical modelis developed to describe the capacitance behavior of nanostructured materials under the combined influence of friction, electric, and magnetic fields. The model uniquely modifies the potential term in the Schrödinger equation using Newtonian mechanics in a frictional environment, thereby coupling quantum and electrochemical phenomena within a unified theoretical framework. The results reveal that both physical parameters (friction coefficient, dielectric constant, magnetic permeability) and chemical factors (ionic composition, doping concentration, and defect chemistry) cooperatively determine nano-capacitance. This theoretical formulation provides a predictive toolfor optimizing the design of high-performance nano-capacitors and energy storage devices, establishing a direct connection between quantum physics and applied electrochemical engineering.

Keywords: Nano materials, Schrödinger equation, Capacitance, Electrochemical behavior, Friction coefficient, Magnetic field, Adsorption, Affinity,

INTRODUCTION

The growing global demand for energy has become one of the most pressing challenges of the modern era. Meeting this need requires the continuous development of energy sources that are both sustainable and environmentally responsible. Among the renewable alternatives, solar energy stands out as one of the most promising; however, its natural intermittency, especially during periods of low sunlight, necessitates efficient and durable energy storage technologies. The most viable approach for storing harvested solar energy is through electrochemical systems, such as rechargeable batteries, which can convert, accumulate, and later release electricity. These batteries not only supply power during non-sunlight hours but also play a critical role in electric mobility, helping reduce total system weight, minimize energy consumption, and enhance operational reliability.

The fast expansion of solar applications and electric vehicles has fueled intense research into advanced energy storage systems. Current investigations are directed toward enhancing several key parameters—storage capacity, cycle

stability, recyclability, and cost effectiveness. To accomplish these objectives, scientists are turning to nanostructured materials, which allow the control of matter at atomic and molecular scales beyond the limits of bulk solids. Nanomaterials exhibit unique physical and chemical behaviors that arise from their reduced dimensions and high surface-to-volume ratio, making them excellent candidates for next-generation storage devices.

Within the scope of nanoscience, which focuses on entities sized from approximately 1 to 300 nanometers, matter behaves in accordance with quantum-mechanical principles rather than classical laws. Adjusting parameters such as crystal geometry, particle size, and atomic arrangement allows tuning of electronic and optical characteristics. Hence, constructing a quantum-based model for nanoscale storage systems is vital to interpret and predict the electrochemical performance, particularly the capacitance, stability, and energy retention. Achieving this goal, however, requires integrating insights from both theoretical frameworks and experimental observations reported in previous studies.

From a chemical perspective, the charge-storage ability of nanomaterials is determined by their crystalline order, surface composition, and structural defects. Variations in ionic substitution, doping level, or oxygen vacancy concentration alter the electronic distribution and local charge density, which consequently influence capacitance. Additionally, surface redox sites at the electrode–electrolyte interface give rise to pseudo-capacitive effects, where reversible ion–electron coupling processes contribute to extra charge storage beyond the ideal double-layer mechanism. These chemical interactions act together with physical variables—such as friction, electric, and magnetic fields—to fully describe the energy-storage dynamics. Therefore, a unified quantum–electrochemical model becomes essential for predicting and optimizing the behavior of nano-capacitors and related systems.

Previous investigations provide important foundations for such modeling approaches. Najwa and collaborators[13], as well as Tayfor[14], reformulated the Schrödinger equation using an energy term derived from Newtonian mechanics, conceptualizing electrons as quantum strings within a friction-affected medium. Their solutions, obtained via Green's function methods, revealed that nanoscale devices can exhibit capacitor-like properties governed by the friction coefficient of the surrounding medium. Similarly, Salma *et al.,*[15,16] demonstrated that nickel-based nanosheets on carbon substrates serve as efficient electrodes in lithium–sulfur batteries due to their enhanced electrochemical performance and charge-storage capacity.

Mashair *et al.,*[17] expanded the concept by incorporating Maxwell's electromagnetic equations with Newtonian mechanics, treating charged particles as oscillating strings, and showed that both friction and oscillation frequency strongly influence capacitance. Ahmed *et al.,*[18] studied Al-doped ZnS thin films and observed notable variations in optical absorption with dopant concentration, suggesting their potential to act as tunable nano-capacitors. Collectively, these works established a theoretical basis for identifying the parameters that control nanoscale charge-storage phenomena.

Recent computational and experimental efforts further highlight the effect of magnetic fields on electrochemical performance. Ruan[19] employed density functional theory (DFT) and molecular dynamics to show that a moderate magnetic field improves lithium-ion mobility and electrode stability by suppressing dendrite formation. Costa[20] confirmed that controlled magnetic exposure enhances ion transport and charge kinetics, thus improving battery capacity and cycling efficiency. Ganguly[21] developed a ferromagnetic anode composed of α-Fe_2O_3 nanoparticles coated with N-doped carbon, achieving superior capacity due to concurrent intercalation and conversion reactions, which were amplified under external magnetic fields. Likewise, Wang[22] and Lee[23] demonstrated that external field-assisted techniques—whether magnetic, optical, or acoustic—can significantly enhance electrochemical kinetics and long-term stability. Nduka[24] verified that incorporating Fe_2O_3 nanoparticles under magnetic processing reduces polarization losses and increases the diffusion coefficient in $LiFePO_4$ cathodes, while Ruan[25] observed measurable improvements in discharge–charge energy in practical 18650-type cells.

Together, these findings emphasize the need for a comprehensive theoretical framework that unites quantum physics with electrochemical

modeling. The present study introduces such an approach to elucidate how both physical and chemical factors influence the capacitance and energy-storage characteristics of nanostructured materials. The subsequent sections of this paper detail the development of the quantum–chemical model (Section 2), its implications and analysis (Section 3), and the key conclusions (Section 4).

Despite significant progress in modeling electrochemical capacitance, existing studies often treat the physical and chemical factors separately. Quantum models typically focus on electron behavior without accounting for frictional and magnetic effects, whereas electrochemical models emphasize material composition but lack quantum-level coupling. No comprehensive theoretical framework has yet unified these two perspectives to describe how both mechanical dissipation and chemical composition jointly control nano-capacitance.

Therefore, the present study aims to bridge this gap by formulating a quantum–electrochemical model that integrates the Schrödinger equation with Newtonian mechanics in a frictional medium under external fields. This unified approach establishes a predictive link between quantum parameters (wave function, potential energy) and measurable electrochemical properties, providing a solid theoretical basis for designing advanced nano-scale energy storage devices.

Quantum–Chemical Nano Model for Electric Capacitance

To formulate a quantum–level description of capacitance in nanostructured materials, the starting point is the time-independent Schrödinger equation, which is modified to incorporate both physical and chemical influences within the potential function. The model considers a charged particle—such as an electron or ion—moving through a dissipative (frictional) medium subjected to an external electric potential (V) and a magnetic field (B). The potential energy in this case is obtained from Newton's second law, which includes terms representing the electric field, magnetic contribution, and damping due to friction. This extended framework enables the Schrödinger equation to simultaneously represent mechanical, electrical, and magnetic interactions within the same physical system[27].

From a chemical viewpoint, the ionic composition, lattice imperfections, and doping concentration of the material alter both the charge density (ρ) and the dielectric constant (ε). According to Gauss's law, variations in these properties affect the local electric field distribution, and therefore modify the material's overall capacitance. Additionally, the collective oscillations of ions and electrons (phonons) are coupled to surface redox reactions, which contribute to pseudo-capacitance.

Solving the Schrödinger equation with this modified potential yields a complex wave number, where the real part represents electrostatic contributions, while the imaginary part corresponds to damping and energy losses from friction and ion–phonon coupling. This establishes a direct relationship between the quantum state of charge carriers and the electrochemical performance of the nanomaterial, providing a predictive basis for engineering enhanced capacitance. The general form of the Schrödinger equation is

$$-\left(\frac{\hbar^2}{2m}\right)\nabla^2\psi + V\psi = E\psi \tag{1}$$

Here, E denotes the total energy of the system, and the potential V accounts for both external fields (electric and magnetic) and chemical effects such as dopant concentration and defect distribution, which determine ε and ρ.

For a charged particle in a frictional medium, Newton's second law can be written as:

$$m\frac{dv}{dt} = -\frac{dV}{dx} - \gamma v + Bev \tag{2}$$

where γ represents the friction coefficient linked to carrier scattering by impurities and defects, and qE depends on the material's ionic density and crystal composition.

The instantaneous displacement between positive and negative charges can be expressed as

$$d = d_0 e^{-i\omega t} \tag{3}$$

This harmonic oscillation of amplitude d_0 and frequency ω describes lattice vibrations and ionic responses to the applied field. Doping or the presence of oxygen vacancies modifies the lattice stiffness and therefore alters d_0, establishing a

chemical coupling between the lattice structure and the electrochemical behavior of the material.

For a medium containing periodic arrays of ions and electrons, the electric potential is generated as the system behaves like a capacitor that sustains a uniform field E. By applying Gauss's law, the relation between charge and electric flux density D is:

$$\int_{-ve}^{+ve} D \bullet dA = \varepsilon \int E \bullet dA = Q = \sigma_e A \tag{4}$$

For the positive electrode:

$$E^+ = \frac{\sigma_e}{\varepsilon}$$

and for the negative electrode:

$$E_- = -\frac{\sigma_e}{\varepsilon} \tag{5}$$

The total electric field across the capacitor becomes:

$$E = E^+ - E^- = \frac{2\sigma_e}{\varepsilon} = E_0 \tag{6}$$

This field depends on the surface charge density σ_e, which is directly related to the defect chemistry and ionic distribution of the nanomaterial. The oscillation of ions and electrons leads to a time-varying potential:

$$V_e = \underline{E_0}\underline{d} = E_0 d_0 \, e^{\wedge}(-i\omega t) = V_0 e^{-i\omega t} \tag{7}$$

Hence, the potential can be represented as:

$$V = V_0 e^{-i\omega t} = V_f \tag{8}$$

This oscillatory form corresponds to dynamic charge exchange processes and redox interactions occurring at the interface, which are the source of pseudo-capacitive effects.

Considering the equation of motion under the oscillatory potential V_f:

$$m\frac{dv}{dt} = -\frac{1}{v}\frac{dV_f}{dt} - \gamma v + Bev \tag{9}$$

Multiplying both sides by v gives:

$$m \int v dv = -\int dV_f - \gamma \int v^2 \, dt + \beta e \int e^v \, dt + C_0 \tag{10}$$

Define for simplicity:

$$\gamma_0 = \gamma - \beta_e \tag{11}$$

Integrating equation (10):

$$\tfrac{1}{2}mv^2 + V_f = \left(\frac{\gamma^0}{2i\omega}\right) v_0^2 e^{-2i\omega t} + C_0 \tag{12}$$

Rearranging yields the constant of motion:

$$\tfrac{1}{2} m v^2 + V_f + \frac{i\gamma_0 v^2}{2\omega} = C_0 = E \tag{13}$$

Hence, the total energy is expressed as:

$$E = \tfrac{1}{2} m v^2 + V_f + \left(\frac{i\gamma_0 v^2}{2\omega}\right) \tag{14}$$

The classical Newtonian form of energy is:

$$E = \tfrac{1}{2}mv^2 + V \tag{15}$$

By comparing (14) and (15), the effective potential becomes:

$$V = V_f + \left(\frac{i\gamma_0 v^2}{2\omega}\right) \tag{16}$$

This potential incorporates the field energy along with damping and magnetic effects. Substituting into the Schrödinger equation:

$$-\left(\frac{\hbar^2}{2m}\right)\nabla^2\psi + V\psi = E\psi \tag{17}$$

Substituting (16) into (17):

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \left(V_f + \frac{i\gamma_0 v^2}{2\omega}\right)\psi = E\psi \tag{18}$$

Assuming uniform potential:

$$V_f = V_0 \tag{19}$$

The wave function solution is:

$$\psi = Ae^{ikx} \tag{20}$$

A direct substitution of (20) in (18) gives

$$\frac{\hbar^2 k^2}{2m} + V_0 + \frac{i\gamma_0 v^2}{2\omega} = E \tag{21}$$

Hence

$$\frac{\hbar^2 k^2}{2m} = (E - V_0) - \frac{i\gamma_0 v^2}{2\omega} \tag{22}$$

The structure of (22) requires the wave number to be complex, such that

$$k = k_1 + ik_2 \tag{23}$$

$$\hbar^2(k_1^2 - k_2^2 - 2ik_1k_2) = 2m(E - V_0) - \frac{i\gamma_0 v^2}{\omega} \tag{24}$$

Equating the imaginary parts on both sides of the above relation gives

$$2k_1 k_2 = \frac{-\gamma_0 m v^2}{(\hbar^2 \omega)} \tag{25}$$

Since the electron is accelerated by the electric potential it follows that the gained kinetic energy is given to be

Thus equation (24) gives

$$k_2 = -\frac{\gamma_0 (m v^2)}{(2\hbar^2 \omega\, k_1)} \tag{26}$$

The current density J can be defined in terms of the number density n which is related to the square of the modules of the wave function, beside the speed v and the electronic charge e to be

$$J = ne\, v = e\, v\, |\psi|^2 \tag{27}$$

Thus according to equations (20,23) one gets

$$J = e\, v\, A^2 e^{-2k_2 x} \tag{28}$$

for very small tiny nano particle of dimensions a

$$x \approx a \tag{29}$$

thus

$$J = e\, v\, A^2 e^{-2k_2 \alpha} \tag{30}$$

Since a is extremely small, thus for the vase when

$$2k_2\alpha \ll 1 \tag{31}$$

Equation (30) reduced to

$$J = e\, v\, A^2 (1 - 2k_2\alpha) \tag{32}$$

Hence from equation (26)

$$J = e\, v\, A^2 \left[1 + \frac{\gamma_0 m v^2}{(\hbar^2 \omega k_1)} \right] \tag{33}$$

The charge density n is chemically dependent, varying with doping concentration and ionic substitution, and directly affects the current density.

$$v = w r_0 \tag{34}$$

A direct insertion of (34) in (33) gives

$$J = ne\, \omega\, r_0 A^2 \left(1 + \frac{\gamma_0 m\, r_0^2 \omega}{\hbar^2 k_1} \right) \tag{35}$$

$$J = \frac{ne\hbar w}{\hbar} \left(1 + \frac{\gamma_0 m\, r_0^2 \omega}{\hbar^2 k_1} \right) \tag{36}$$

The amplitude r_0 reflects lattice vibrations, which are influenced by chemical composition and structural defects.

$$eV = E = h\omega \tag{37}$$

$$J = ne^2 r_0^2 A^2 \left(1 + \frac{\gamma_0 m\, r_0^2 \omega}{\hbar^2 k_1} \right) V \tag{38}$$

$$J = Y\, V \tag{39}$$

This relation resembles current–voltage characteristics in electrochemical capacitors, linking quantum mechanics with electrochemical performance.

$$J = \omega\, c\, V 2\, k_1 k_2 = \frac{-\gamma_0 m\, r_0^2 \omega}{(\hbar^2 k_1)} k_2 = -\frac{\gamma_0 (m\, r_0^2 \omega)}{(2\, \hbar^2 \omega\, k_1)} \tag{40}$$

Thus, the capacitance according to equations (11), (38), (40) is given by:

$$C = ne^2 r_0^2 A^2 \left(\frac{1}{\omega} + \frac{(\gamma_0 m\, r_0^2)}{(\hbar^2 k_1)} \right)$$

$$= ne^2 r_0^2 A^2 \left(\frac{1}{\omega} + \frac{((\gamma + BE) m\, r_0^2)}{(\hbar^2 k_1)} \right) \tag{41}$$

This expression shows capacitance depends on dielectric constant ε, carrier density n, and structural damping, all influenced by the chemical environment of the nano material.

$$E = \frac{1}{2} C V^2 \tag{42}$$

This quantum–chemical model therefore shows that both physical parameters (friction, electric and magnetic fields) and chemical factors (composition, doping, and surface structure) cooperatively determine the capacitance and energy-

storage efficiency of nanomaterials.Thus according to equations (41) and (42). The applied magnetic field density (B) is related to both capacitance (C) and energy stored (E). Accordingly, can be displayed graphically using simulation as shown in Figures (1) and (2).
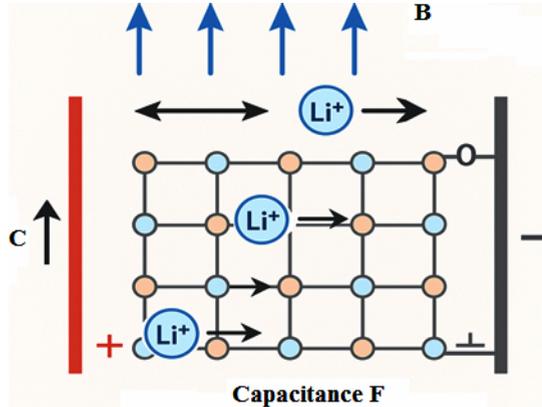

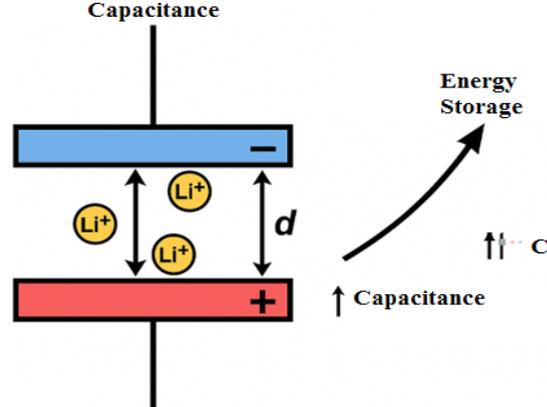**Fig. 1. Schematic representation of the influence of an external magnetic field (B) on the capacitance (C) of a nano-capacitor. The applied magnetic field enhances Li* ion mobility within the lattice, improving charge transport and increasing capacitance. This illustrates the direct coupling between magnetic-field-induced quantum behavior and electrochemical ion dynamics**

Fig. 2. Graphical relationship between capacitance (C) and stored energy (E) in a nano-capacitor. As Li* ions accumulate at the electrode–electrolyte interface, the increase in capacitance results in a proportional enhancement in stored energy, demonstrating the electrochemical–quantum coupling predicted by the theoretical model.
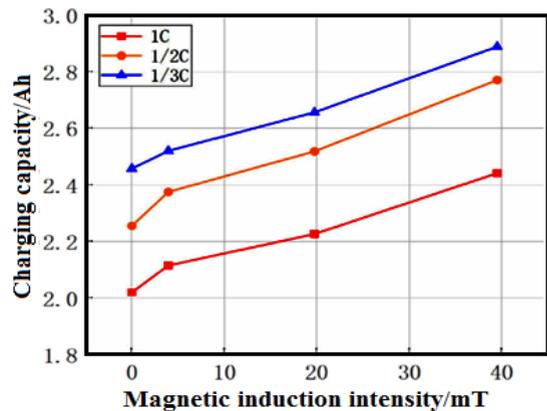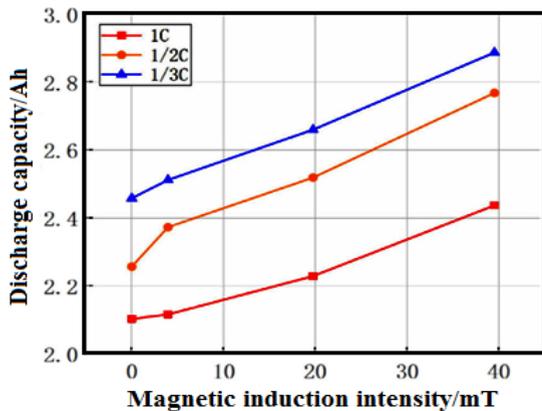

Fig. 3(a). Discharge capacity curve of battery at different rates; (b) Charge capacity curve of battery at different rates[25]
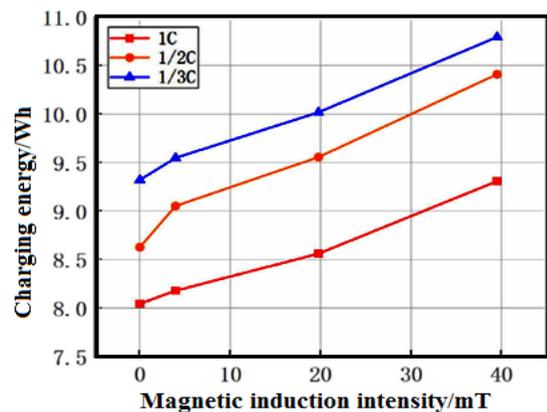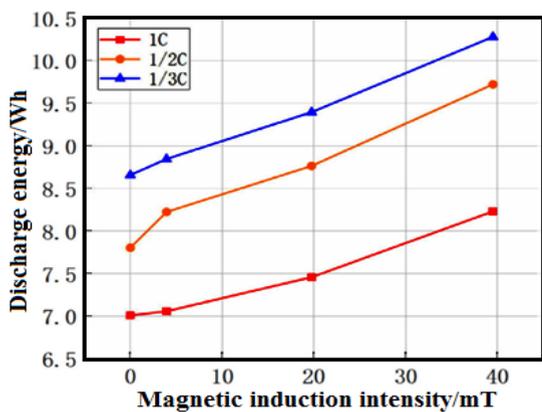

Fig. 4(a). Discharge energy curve of battery at different rates; (b) Charge energy curve of battery at different rates[25]
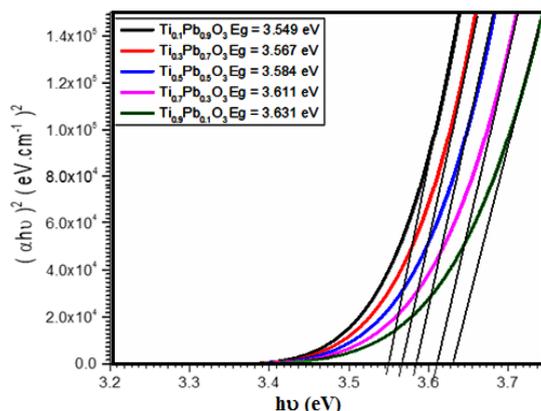
Fig. 5). Optical energy band gaps of (Ti$_x$Pb$_{1-x}$ O$_3$) samples[26]

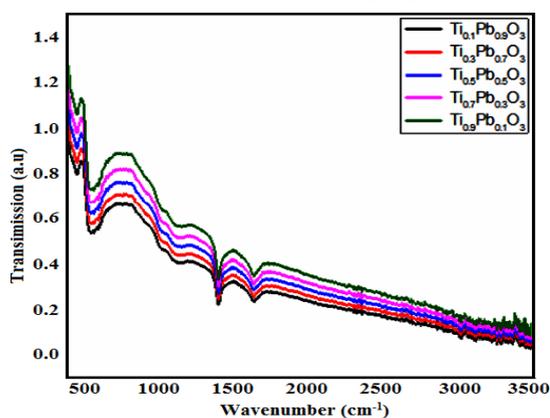**Fig. 6. FTIR spectrum of all (Ti$_x$Pb$_{1-x}$O$_3$) samples[26]**

Table 1: FTIR chemical bonds of all samples that meade by (Ti$_x$Pb$_{1-x}$O$_3$)[26]

Wave number (cm^{-1})	Fuction groups	Viberation
461	metal-oxygen	Pb-O
549	Alken sp^2	C-H cis
1400	Bend sp^3	C-H stretch
1640	Alken	C=C stretch
3470	Water	O-H stretch

DISCUSSION

The proposed quantum–chemical framework offers a deeper understanding of how both physical and chemical parameters govern the capacitance behavior of nanostructured materials. By formulating a potential energy term derived from Newtonian mechanics for a frictional medium and integrating it into the Schrödinger equation, the model demonstrates that the capacitance is influenced by the friction coefficient, the intensity of the applied electric and magnetic fields, and the intrinsic dielectric properties of the material.

From a chemical standpoint, the dielectric permittivity (ε) is strongly dependent on the ionic configuration, defect density, and dopant concentration within the crystal lattice. Substitutional doping—such as the incorporation of aluminum or iron atoms—modifies the lattice polarizability, which consequently alters the charge carrier density (n) and the real component of the wave number (k$_1$). The imaginary component (k$_2$), on the other hand, is closely associated with scattering phenomena resulting from lattice defects and impurities, linking the damping term directly to the degree of disorder in the material. Furthermore, variations in band gap energy caused by the doping process are correlated with changes in electron affinity, while FTIR spectral observations confirm that doping influences the adsorption behavior of the material—both of which are essential for describing the electrochemical response.

The oscillatory potential term included in the theoretical model can be interpreted as a representation of surface redox activity occurring at the electrode–electrolyte interface. These reversible ion–electron exchange processes contribute to pseudo-capacitance, a well-recognized electrochemical mechanism that enhances charge storage beyond the ideal double-layer behavior. Consequently, the quantum–mechanical analysis presented in this study is in excellent agreement with experimentally observed electrochemical features of advanced energy storage systems.

The effect of the magnetic field on capacitance also finds chemical justification. Increasing the magnetic field intensity promotes the movement of Li* and other mobile ions by facilitating convective and diffusive transport, thereby enhancing overall ionic conductivity. This explanation aligns with experimental studies on magnetic-field-assisted lithium-ion batteries, which report improved ion mobility, reduced dendrite formation, and extended cycle life when external fields are applied.

Finally, the analytical expression for capacitance derived in Eq. (41) clearly shows that energy storage performance is a multifactorial phenomenon, controlled by both physical and chemical parameters.

- Physical contributions: friction coefficient, oscillation frequency, and applied field intensity.
- Chemical contributions: ionic concentration, lattice defect structure, dopant level, and redox activity at material interfaces.

Overall, the developed model successfully integrates quantum physics with electrochemical theory, offering a unified predictive platform for designing and optimizing nano-capacitors and other high-performance energy storage materials. This integration highlights the possibility of tuning capacitance through the combined adjustment of both external physical conditions and internal chemical composition, bridging the gap between theoretical modeling and practical material design.

CONCLUSION

In this study, a comprehensive quantum–chemical model was formulated to explain the capacitance behavior of nanostructured materials. The model was established by solving the Schrödinger equation containing a potential term derived from Newtonian mechanics for a frictional environment influenced by both electric and magnetic fields. The theoretical framework reveals that the capacitance is governed not only by physical parameters—such as the friction coefficient, oscillation frequency, and field intensity—but also by chemical characteristics including ionic configuration, dopant concentration, and lattice defect structure.

The oscillatory potential employed in the model reflects the dynamic coupling between electrons and ions, which is directly associated with electrochemical processes such as pseudo-capacitance arising from surface redox interactions. The inclusion of dielectric permittivity (ε) and charge density (ρ) parameters emphasizes the decisive roles of chemical composition and crystal imperfections in determining the overall storage capability of the nanomaterial.

Moreover, variations in doping concentration were found to influence both electron affinity and adsorption behavior, indicating that electronic and chemical modifications can be utilized to enhance energy storage efficiency. The derived relations clearly demonstrate that the capacitance and stored energy can be systematically controlled through a coordinated adjustment of physical conditions and chemical composition.

Hence, the developed model provides a predictive and unified theoretical platform for designing high-performance nano-capacitors and advanced electrochemical energy storage devices, effectively bridging the conceptual gap between quantum physics and electrochemical engineering.

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