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Quantum Modelling of Hydroxyl Topology Control of the Stokes-Induced Stark Effect in Hybrid Flavonoid–Semiconductor Interfaces

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ABSTRACT

The Stokes-Induced Stark Effect (SISE) has recently been identified as a novel mechanism for generating localized electric fields at hybrid photoactivated molecular–semiconductor interfaces, yet the structural factors governing its magnitude remain unresolved. Here, we develop a quantum-mechanical framework demonstrating that the strength of SISE is quantitatively controlled by the hydroxyl topology of flavonoid chromophores through excited-state intramolecular proton transfer (ESIPT). ESIPT induces transient charge redistribution and dipole amplification, which act as the primary source of the interfacial electric field. Using a Rosen–Morse II potential, the framework provides a dual-regime description of the interface, comprising a global bound-state formulation and a local Airy-type reduction for strong-field behavior. A hydroxyl-topology descriptor Ω_{OH} , constructed from excited-state dipole change, molecular orientation, and interfacial separation, is introduced to capture the ESIPT-mediated structural dependence and is applied to a series of flavonoids (myricetin, quercetin, kaempferol, luteolin, and curcumin). The results show that SISE-induced energy shifts follow distinct scaling laws, with $\Delta E_n \propto \Omega_{\text{OH}}^2$ in the global regime and $E_n \propto \Omega_{\text{OH}}^{2/3}$ in the local regime, accompanied by a transition from symmetric confinement to field-driven localization. The analysis further identifies the B-ring pyrogallol configuration as the optimal architecture for maximizing SISE, while ESIPT-inactive systems define a limiting case with suppressed field generation. This work establishes the first quantitative structure–field relationship for SISE, providing a predictive basis for the molecular design of field-tunable hybrid optoelectronic interfaces.

Stokes-Induced Stark Effect (SISE), hydroxyl topology, excited-state intramolecular proton transfer (ESIPT), flavonoids, interfacial electric field

1.0. INTRODUCTION

The global technological and industrial shift toward hybrid organic–inorganic semiconductor systems is reshaping modern electronics, enabling new generations of optoelectronic, photocatalytic, molecular electronic, and bioelectronic technologies. In these hybrid materials, organic chromophores are coupled with inorganic semiconductors to create interfaces where electronic excitations, charge transfer, and interfacial electric fields govern device performance and catalytic activity[1-3]. Electric-field–induced modulation of electronic states, termed the Stark effect, plays a critical role in regulating charge-transfer states, excitonic energies, and fluorescence behavior at such interfaces[4-6]. Recent studies have further demonstrated that

electric fields can control electron transport and electronic coupling across molecule–semiconductor junctions, highlighting the central role of interfacial electrostatics in hybrid materials[7-8]. However, in most existing frameworks these fields are treated either as externally applied biases or as static interfacial parameters. The fundamental challenge therefore remains the lack of a mechanism by which such electric fields can be generated and controlled intrinsically through molecular design.

Naturally occurring hydroxyl-rich flavonoids provide a promising molecular architecture for addressing this challenge. These chromophores exhibit complex photophysical behavior characterized by large Stokes shifts and excited-state intramolecular proton transfer (ESIPT) processes that drive rapid redistribution of electronic charge on ultrafast timescales [9-11]. Such excited-state dipole reorganizations suggest that the electronic relaxation accompanying Stokes emission may generate transient electric fields capable of perturbing the electronic states of a nearby semiconductor. In this context, we have previously introduced the Stokes-Induced Stark Effect (SISE), defined as the generation of a localized electric field (E_{loc}) arising from excited-state dipole reorganization following Stokes relaxation, which subsequently induces Stark modulation of the electronic energy levels of an adjacent semiconductor[12]. Understanding how such molecularly generated electric fields arise and how their magnitude can be systematically controlled through the topology of hydroxyl groups in flavonoid chromophores has therefore become an urgent problem as hybrid organic–inorganic systems continue to expand into applications ranging from photocatalysis to bioelectric materials.

Despite growing recognition of electric-field effects in hybrid molecular–semiconductor systems, the factors governing the magnitude of such fields at the molecular level remain poorly understood. Stark spectroscopy studies have demonstrated that electric fields can modulate fluorescence spectra and electronic energy levels in molecular systems [4,13], while semiconductor physics has established that interfacial electric fields regulate charge-transfer states and excitonic energies at organic–inorganic interfaces [5,6,8,14]. At the molecular scale, extensive investigations of flavonoid photophysics have shown that hydroxyl substitution patterns strongly influence excited-state intramolecular proton transfer, charge redistribution, and fluorescence behavior in flavonol chromophores[10,11,15]. Complementary studies have further demonstrated that hydroxyl groups can mediate interfacial charge-transfer dynamics and photocatalytic activity on semiconductor surfaces [16-20]. Building on these insights, recent theoretical work has introduced the Stokes-Induced Stark Effect (SISE), demonstrating that excited-state dipole reorganization following Stokes relaxation in flavonoid–semiconductor systems can generate localized electric fields capable of modulating semiconductor electronic states[12]. However, while the SISE mechanism establishes the existence of molecularly generated Stark fields, the structural determinants governing the strength of this effect remain unknown. In particular, there is no systematic framework that currently explains how the number, spatial arrangement, and electronic coupling of hydroxyl groups within flavonoid structures, collectively referred to as hydroxyl topology control the magnitude of the Stokes-induced electric field and the resulting Stark modulation at hybrid interfaces. Thus, the relationship between hydroxyl architecture and SISE strength remains an unresolved problem in hybrid organic–inorganic semiconductor physics.

Here, we fill this gap by proposing that hydroxyl topology controls the strength of the Stokes-Induced Stark Effect in hybrid flavonoid–semiconductor interfaces. Specifically, we hypothesize that the number, spatial arrangement, and electronic coupling of hydroxyl groups within flavonoid molecules regulate the magnitude of excited-state dipole reorganization during Stokes relaxation, thereby determining the strength of the localized electric fields responsible for Stark modulation at semiconductor interfaces. To investigate this hypothesis, we develop a Quantum Mechanical framework that integrates molecular photophysics, Stark-effect theory, and interfacial electrostatics, and apply it to a representative series of hydroxylated flavonoids viz myricetin, quercetin, kaempferol, luteolin, and curcumin, whose molecular structures span a wide range of hydroxyl configurations. Within this framework, we introduce a hydroxyl-topology descriptor that quantifies the contribution of hydroxyl groups to Stokes-induced electric-field generation and enables systematic comparison of SISE strength across different flavonoid architectures. This direction is motivated by growing evidence that functional groups can regulate electronic coupling and charge dynamics in hybrid organic–inorganic semiconductor systems[19,21-24], as well as recent theoretical demonstrations that plant-derived chromophores can participate in field-mediated excitonic processes at semiconductor interfaces[12,14, 25-26]. By establishing a mechanistic relationship between hydroxyl topology, excited-state photophysics, and interfacial Stark modulation, this work provides a predictive framework for controlling electric-field–driven phenomena in hybrid molecular–semiconductor materials and opens new possibilities for designing bioinspired optoelectronic, photocatalytic, and bioelectric systems.

2.0. METHODS

2.1. Description of Hydroxyl Topology at Flavonoid-Semiconductor Interface

The hydroxyl group constitutes the primary molecular degree of freedom linking flavonoid excited-state photophysics to interfacial electrostatics in SISE-active hybrid systems. In 3-hydroxyflavone derivatives, an intramolecular hydrogen bond between the 3-hydroxyl and carbonyl oxygen enables excited-state intramolecular proton transfer (ESIPT) following photoexcitation, driving a transition from the normal excited state (N^*) to a tautomeric state (T^*) with strongly redistributed charge density[9,10,11,15]. This ultrafast reorganization produces a substantial dipole moment change ($\Delta\mu$), typically on the order of several Debye, as confirmed by spectroscopic and theoretical studies[27-28]. The resulting time-dependent dipole constitutes the microscopic origin of the localized electric field generated during Stokes relaxation, as illustrated in Figure 1. The magnitude and directionality of this dipole response are governed by hydroxyl topology through its control of π -conjugation and charge-transfer pathways. Hydroxyl groups positioned on the B-ring, particularly in 3',4' catechol configurations, enhance donor–acceptor coupling between the phenolic ring and the chromone core, thereby increasing excited-state polarization[29-31]. In contrast, hydroxyl groups outside the conjugation pathway or deviating from coplanarity contribute weakly due to reduced π -orbital overlap[32]. Thus, the effective dipole change is determined not simply by hydroxyl count but by their spatial arrangement and electronic connectivity. The interfacial configuration responsible for this coupling is shown in Figure 2, where the flavonoid is chemisorbed onto the semiconductor surface through the ESIPT-active anchoring site.

Molecular Mechanism of 3-hydroxyflavone ESIPT and Stokes Shift

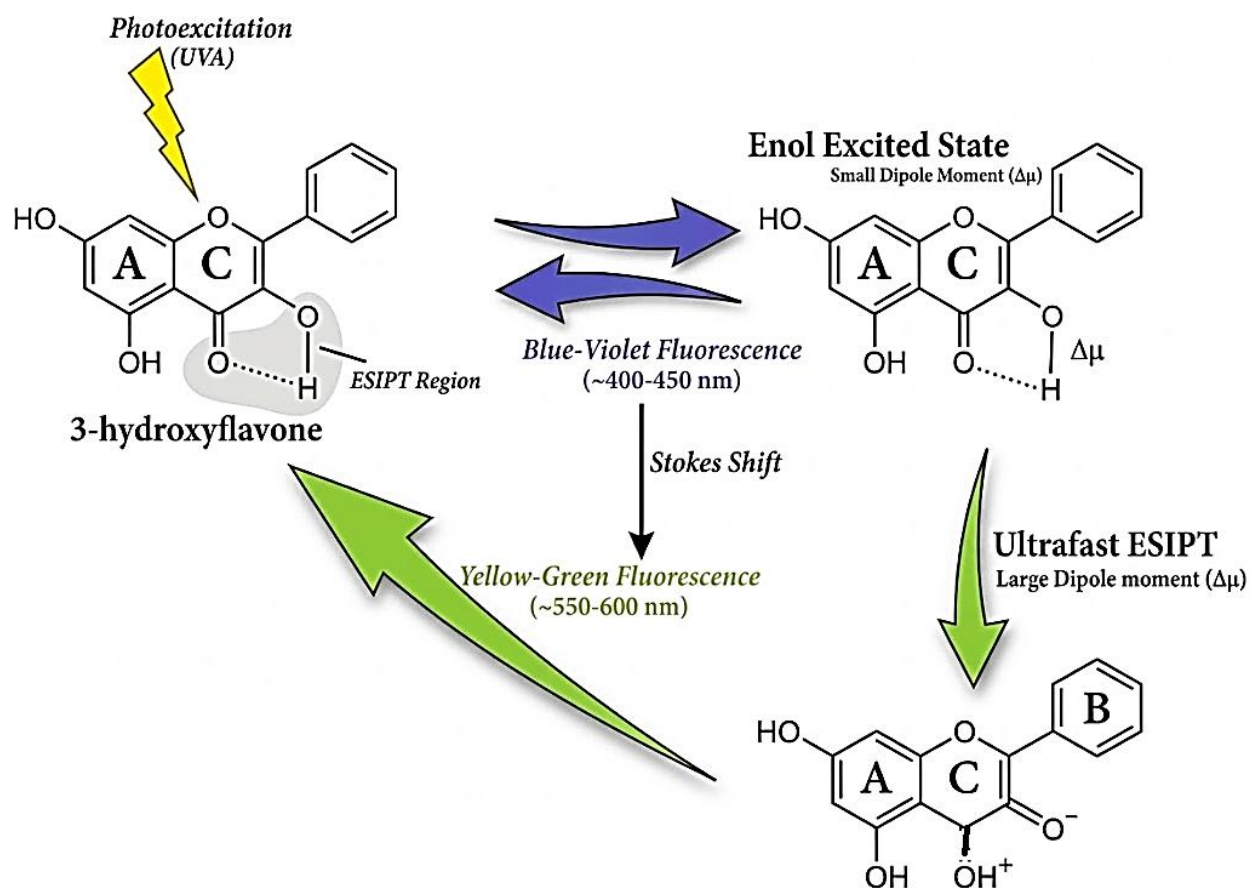


Figure 1 | Excited-State Intramolecular Proton Transfer (ESIPT) and Stokes-Shift Photophysics in 3-Hydroxyflavone

This schematic illustrates the photophysical sequence following ultraviolet photoexcitation in 3-hydroxyflavone, the prototypical ESIPT chromophore. In the ground state (S₀), the molecule exists in its enol configuration stabilized by an intramolecular O-H...O hydrogen bond. Absorption of a UVA photon promotes the molecule into the Franck-Condon enol excited state (N*), which emits blue-violet fluorescence (~420–450 nm). Ultrafast ESIPT (<1 ps) transfers the proton to form the keto excited state (T*), leading to a substantial increase in dipole moment (Δμ) and a red-shifted yellow-green Stokes emission (~550–600 nm). The enol-to-keto tautomerization, coupled with the associated dipole moment jump, constitutes the fundamental molecular process underlying transient electric field generation. This dipole-driven field evolution provides the physical basis for the Stokes-Induced Stark Effect (SISE) when the molecule is interfaced with a semiconductor surface.

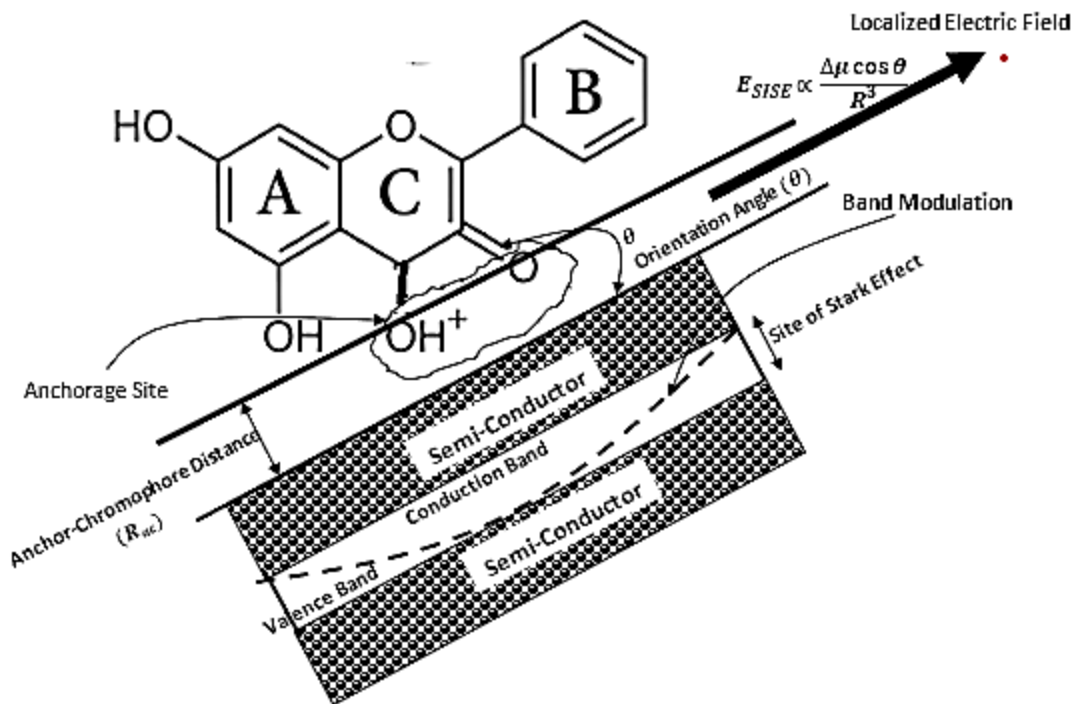


Figure 2|Chemisorption Geometry and Stokes-Induced Stark Field Generation at the Flavonoid–Semiconductor Interface

This schematic illustrates the interfacial configuration responsible for Stokes-induced electric field generation in a flavonoid–semiconductor hybrid system. Following excited-state intramolecular proton transfer (ESIPT), the flavonoid adopts a polarized keto-like excited state characterized by a large dipole moment ($\Delta\mu$). The molecule chemisorbs onto the semiconductor surface through the ESIPT-active carbonyl–hydroxyl coordination site, forming a stable anchoring geometry that positions the chromophore at a finite anchor–surface distance R_{ac} . The molecular dipole is oriented at an angle θ relative to the semiconductor surface, defining the projection of the dipole along the surface normal. This geometric configuration determines the magnitude of the localized electric field generated at the interface, given by $E_{\perp} \propto \Delta\mu \cos \theta / R^3$, where only the perpendicular component contributes to interfacial electrostatic coupling. The generated field penetrates the semiconductor, inducing a Stark shift in the electronic energy levels at the interface. The semiconductor is represented with its valence and conduction bands, which undergo modulation in response to the localized field. The region directly beneath the adsorption site is identified as the locus of the Stark effect, where band bending and energy level shifts occur. This coupling between excited-state dipole reorganization and interfacial electrostatics establishes the physical basis of the Stokes-Induced Stark Effect (SISE), linking molecular photophysics to semiconductor electronic modulation through hydroxyl-mediated chemisorption and geometric alignment.

At the semiconductor interface, hydroxyl groups further act as anchoring sites that define molecular orientation and coupling to the surface as shown in figure 2. Deprotonated or hydrogen-bonded hydroxyls coordinate to surface metal centers on ZnO or TiO₂, forming adsorption geometries that fix the dipole orientation relative to the interface[17,18,33–34]. This geometry determines both the dipole–surface separation R and the projection angle θ , such that the effective interfacial electric field scales as $E_{\perp} \propto \mu \cos \theta / R^3$. Only the perpendicular component contributes to Stark modulation of interfacial electronic states, consistent with established models of hybrid charge-transfer systems[4,5]. Consequently, small variations in hydroxyl positioning can produce significant variations in interfacial field strength.

These coupled roles viz ESIPT activation, conjugation control, orientational alignment, and distance regulation collectively define hydroxyl topology, which governs the generation and coupling of molecular electric fields in SISE-active systems. The selected flavonoids (myricetin, quercetin, kaempferol, luteolin, and curcumin) whose structures are shown in figure 3 span a broad range of hydroxyl configurations, enabling systematic evaluation of topology-dependent effects. Variations in hydroxyl number and placement modulate ESIPT activity, excited-state polarization, and interfacial coupling, providing a chemically controlled platform for probing SISE strength[35-37].

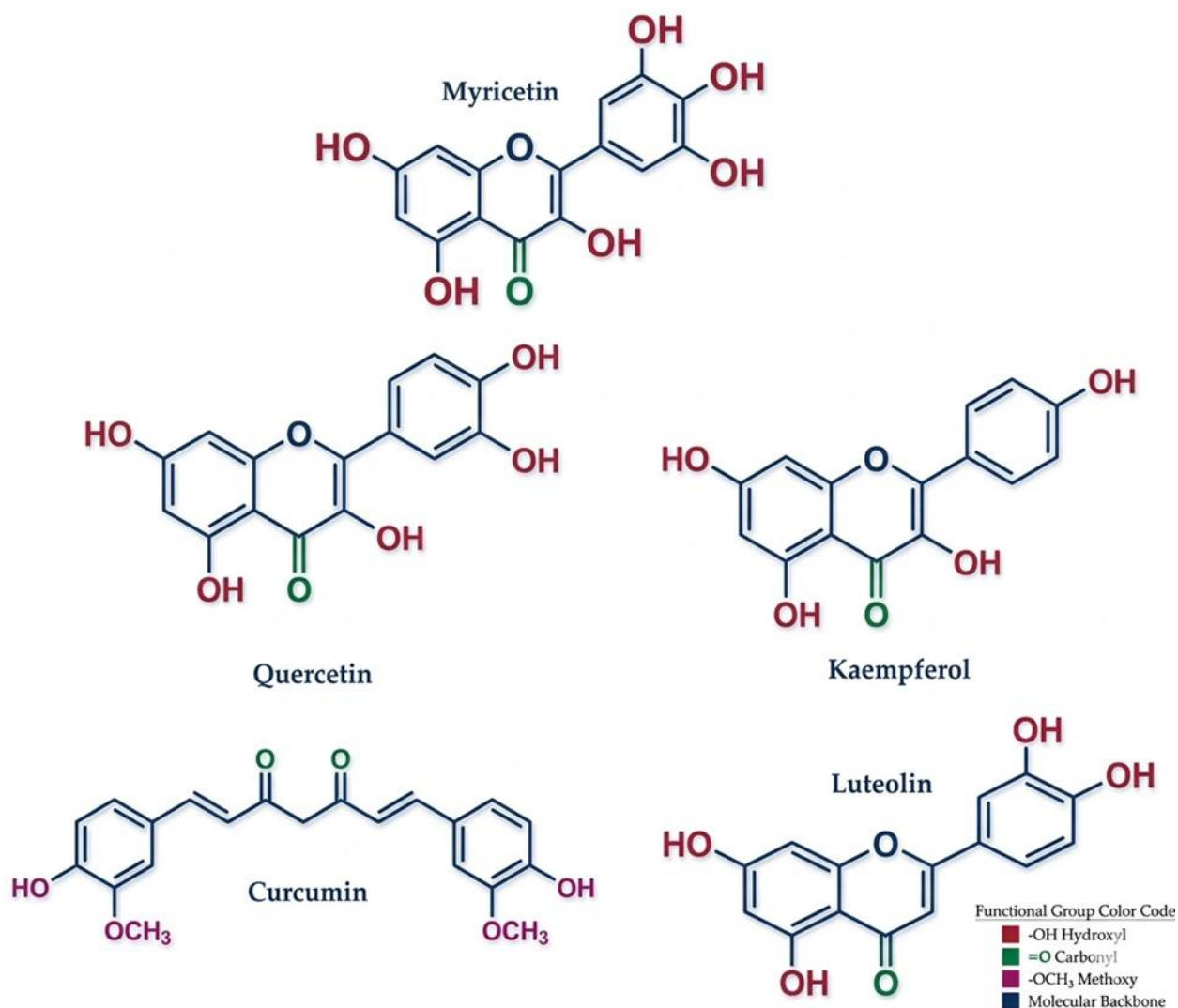


Figure 3 | Molecular structures of selected flavonoids illustrating hydroxyl topology.

Figure 3 presents the structures of myricetin, quercetin, kaempferol, luteolin, and curcumin, highlighting the number and spatial arrangement of hydroxyl groups. These molecules span a range of hydroxyl topologies, from the highly substituted pyrogallol system of myricetin to the reduced substitution in kaempferol and the ESIPT-inactive luteolin. This structural diversity provides a controlled platform for probing the relationship between hydroxyl configuration, excited-state dipole generation, and SISE strength.

At hybrid interfaces, hydroxyl-mediated adsorption introduces additional physical effects, including partial deprotonation, dielectric screening, conformational restriction, and possible orbital hybridization with surface states[17,33,34]. These effects modify both the magnitude and spatial distribution of the induced electric field and are incorporated here through parametrization based on experimental and

computational studies rather than explicit atomistic simulation. These parameters are summarized in table 1 for all 5-flavonoids of interest.

Table 1. Hydroxyl topology and key photophysical parameters of selected flavonoids

Flavonoid	Hydroxyl Positions	ESIPT Active	$\Delta\mu$ (D)	Stokes Shift (cm ⁻¹)	Key Structural Feature	Sources
Myricetin	3,5,7,3',4',5'	Yes (3-OH)	12–15	8000–10000	B-ring pyrogallol (max coupling)	[29,30,35]
Quercetin	3,5,7,3',4'	Yes (3-OH)	10–13	7000–9000	Catechol + ESIPT	[9,28]
Kaempferol	3,5,7,4'	Yes (3-OH)	7–10	6000–8000	Reduced B-ring coupling	[38,39]
Luteolin	5,7,3',4'	No	4–6	3000–5000	No 3-OH → no ESIPT	[29,30,37]
Curcumin	Phenolic OH (2)	Yes (enol)	8–11	5000–7000	β -diketone ESIPT	[40-41]

To capture these processes, we employ a parametrized quantum-mechanical framework based on the time-independent and time-dependent Schrödinger equations. Ground-state properties, including dipole moments and molecular geometries, are obtained from crystallographic and spectroscopic data[28,35,42-43]. Excited-state dynamics are described using a reduced two-state ESIPT model[27,44], where the dipole evolves as:

$$\mu(t) = \mu_g + \Delta\mu \left(1 - e^{-\frac{t}{\tau_{\text{ESIPT}}}} \right) \quad (1)$$

with τ_{ESIPT} in the femtosecond regime[27,45]. The resulting dipole generates a localized interfacial electric field:

$$E_{\perp}(t) = \frac{2\mu(t) \cos \theta}{4\pi\epsilon_0\epsilon_r R^3} \quad (2)$$

where R , θ , and ϵ_r are parametrized from adsorption geometries and interfacial dielectric properties[5,33,34]. This field perturbs semiconductor electronic states via the Stark effect defined as:

$$\Delta E_{\text{Stark}}(t) = -\Delta\mu_{\text{sc}} E_{\perp}(t) - \frac{1}{2} \alpha_{\text{sc}} E_{\perp}(t)^2 \quad (3)$$

consistent with established Stark-effect formalisms for hybrid interfaces[5,7].

This hierarchical formulation combining TISE-based parametrization, TDSE-inspired dipole dynamics, and perturbative interfacial coupling captures the full sequence of SISE generation from molecular excitation to semiconductor response. Within this framework, hydroxyl topology emerges as the key structural descriptor controlling the magnitude and directionality of molecularly generated electric fields in hybrid flavonoid–semiconductor systems.

2.2 Derivation of an Analytically Solvable Interfacial Potential for SISE Manifestation

To establish a rigorous quantum-mechanical description of Stokes-Induced Stark Effect (SISE) manifestation at flavonoid–semiconductor interfaces, we formulate an effective one-dimensional

potential $V(z)$ along the surface-normal coordinate z , with the adsorption region centered at $z = z_0$. This reduction is justified by the strong anisotropy of interfacial coupling in hybrid systems, where charge transfer, excitonic localization, and electric-field effects are predominantly governed by the normal component of the electrostatic field [5,7]. The approach is consistent with established treatments of interfacial Stark phenomena in organic–inorganic heterostructures and electroabsorption spectroscopy[4,6].

At the hybrid interface, two competing physical effects govern the electronic landscape viz localized confinement arising from adsorption, hybridization, and excitonic binding[1,2] and directional asymmetry induced by the Stokes-generated electric field originating from excited-state dipole reorganization[4,6,12,36].

To capture both effects within an analytically tractable framework, we adopt the **Rosen–Morse II potential**, given by

$$V(z) = -V_0 \operatorname{sech}^2[\alpha(z - z_0)] + V_1 \tanh[\alpha(z - z_0)] \quad (4)$$

where $V_0 > 0$ characterizes the depth of the interfacial confinement well, α^{-1} is the spatial localization length, and V_1 quantifies the asymmetry induced by the SISE field. The sech^2 term is widely used to represent localized bound states in quantum wells and surface potentials due to its finite depth and smooth spatial decay, making it physically appropriate for modeling adsorption-induced confinement [1,2]. The $\tanh$ term introduces a spatially odd perturbation that mimics the directional effect of an electric field while preserving exact solvability, a feature exploited in quantum Stark problems and asymmetric well models.

From Eq.(2), the perpendicular component of the Stokes-induced electric field is

$$E_{\perp}(t) = \frac{2\mu(t)\cos \theta}{4\pi\epsilon_0\epsilon_r R^3} \quad (5a)$$

At the point of maximal dipole development following ESIPT, this reduces to

$$E_{\text{SISE}}^{(0)} = \frac{2\Delta\mu\cos \theta}{4\pi\epsilon_0\epsilon_r R^3} \quad (5b)$$

where $\Delta\mu$ is determined by hydroxyl topology through ESIPT efficiency and conjugation pathways[9,11]. The asymmetry parameter V_1 in Eq. (4) is therefore defined as

$$V_1 = \lambda E_{\text{SISE}}^{(0)} \quad (6)$$

where λ is an effective coupling constant that incorporates charge, dielectric response, and interfacial screening. This mapping establishes a direct quantitative link between molecular structure and interfacial potential asymmetry, consistent with prior demonstrations that electric fields at hybrid interfaces can be modulated by molecular dipoles and functional groups [8,19]. Thus the Rosen–Morse II potential inherits an explicit dependence on hydroxyl topology through $\Delta\mu$, R , and θ .

For analytical convenience, we recast Eq. (4) in standard Rosen–Morse form,

$$V(z) = -A(A + 1)\alpha^2 \operatorname{sech}^2[\alpha(z - z_0)] + 2B\alpha \tanh [\alpha(z - z_0)] \quad (7)$$

with

$$V_0 = A(A + 1)\alpha^2, V_1 = 2B\alpha$$

Here, A controls the number of bound states and confinement strength, while B encodes the SISE-induced asymmetry.

The one-dimensional time-independent Schrödinger equation describing the electronic evolution is given as:

$$\left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} - A(A+1)\alpha^2 \operatorname{sech}^2[\alpha(z-z_0)] + 2B\alpha \tanh[\alpha(z-z_0)] \right] \psi(z) = E\psi(z) \quad (8)$$

we introduce the dimensionless coordinate $x = \alpha(z - z_0)$ and define the scaled energy $\epsilon = \frac{2m^*E}{\hbar^2\alpha^2}$ which yields

$$\frac{d^2\psi}{dx^2} + [\epsilon + A(A+1) \operatorname{sech}^2 x - 2B \tanh x] \psi = 0 \quad (9)$$

Following the standard Rosen–Morse transformation, we define

$$y = \frac{1 - \tanh x}{2}, \quad \frac{dy}{dx} = -2y(1-y) \quad 0 < y < 1$$

for which $\tanh x = 1 - 2y$ and $\operatorname{sech}^2 x = 4y(1-y)$.

Substituting into Eq. (9) and applying the chain rule reduces the equation to

$$y(1-y) \frac{d^2\psi}{dy^2} + (1-2y) \frac{d\psi}{dy} + \left[\frac{\epsilon - 2B(1-2y)}{4y(1-y)} + A(A+1) \right] \psi = 0 \quad (10)$$

To remove the singular behavior at $y = 0, 1$, we introduce the ansatz

$$\psi(y) = y^a(1-y)^b f(y) \quad (11)$$

where a and b are chosen to cancel the singular terms at $y = 0$ and $y = 1$

Following standard simplification Rosen–Morse procedure Eq. (11) reduces to the standard Gauss hypergeometric equation

$$y(1-y)f''(y) + [c - (a+b+1)y]f'(y) - abf(y) = 0 \quad (12)$$

The solution is therefore

$$f(y) = {}_2F_1(a, b; c; y) \quad (13a)$$

so the full wavefunction becomes:

$$\psi(y) = y^a(1-y)^b {}_2F_1(a, b; c; y) \quad (13b)$$

For normalizable bound states, the hypergeometric series must terminate $a = -n, n = 0, 1, 2, \dots$

This reduces the solution of Eq. (10) to Jacobi polynomials:

$$\psi_n(x) = (1 - \tanh x)^{\frac{p_n}{2}} (1 + \tanh x)^{\frac{q_n}{2}} P_n^{(p_n, q_n)}(\tanh x) \quad (14)$$

where $P_n^{(p_n, q_n)}$ are Jacobi polynomials and $\mathcal{N}_n$ is a normalization constant. The energy eigenvalues are given by

$$E_n = -\frac{\hbar^2\alpha^2}{2m^*} \left[(A-n)^2 + \frac{B^2}{(A-n)^2} \right], n < A \quad (15)$$

The asymmetry parameter B , which enters explicitly in the energy spectrum, is directly proportional to the Stokes-induced electric field $E_{\text{SISE}}^{(0)}$, thereby establishing a closed analytical link between hydroxyl topology and interfacial Stark-modulated energy levels.

The eigenvalue spectrum in Eq. (15) can be expressed relative to the symmetric case ($B = 0$) as

$$\Delta E_n(B) = E_n(B) - E_n(0) = -\frac{\hbar^2 \alpha^2}{2m^*} \frac{B^2}{(A-n)^2} \quad (16)$$

which defines the SISE-induced correction to the bound-state energies.

Using Eqs.5(b) and (6), the asymmetry parameter is written as

$$B = \frac{\lambda E_{\text{SISE}}^{(0)}}{2\alpha}, \text{ where } E_{\text{SISE}}^{(0)} = \frac{2\Delta\mu \cos \theta}{4\pi\epsilon_0\epsilon_r R^3}$$

so that

$$\Delta E_n = -\frac{\hbar^2}{2m^*} \frac{\lambda^2 (\Delta\mu)^2 \cos^2 \theta}{4(A-n)^2 (4\pi\epsilon_0\epsilon_r R^3)^2} \quad (17)$$

Equation (17) provides the functional dependence of the interfacial energy levels on the molecular dipole change, orientation, and adsorption geometry, and serves as the basis for subsequent analysis.

Local Linear Limit and Airy-Type Reduction

While the Rosen–Morse II potential provides an exact global solution for the interfacial electronic structure, the Stark effect underlying SISE is intrinsically a local field phenomenon. In hybrid organic–inorganic interfaces, field-driven processes such as tunneling, charge separation, and quasi-bound state formation are governed primarily by the local slope of the potential energy landscape rather than its full global form, a standard result in semiconductor heterostructure theory and quantum transport treatments of interfacial fields [5,8 46-47]. Accordingly, a local linearization of the effective potential is appropriate in the vicinity of the classical turning point or an inflection region, where the field contribution dominates over the residual confinement curvature [48-49].

To capture this regime analytically, we expand the interfacial potential $V(z)$ about a reference point $z = z_c$:

$$V(z) \approx V(z_c) + \left. \frac{dV}{dz} \right|_{z_c} (z - z_c) \quad (18)$$

For the Rosen–Morse II potential defined in Eq. (4), the first derivative is

$$\frac{dV}{dz} = 2\alpha V_0 \operatorname{sech}^2[\alpha(z - z_0)] \tanh[\alpha(z - z_0)] + \alpha V_1 \operatorname{sech}^2[\alpha(z - z_0)] \quad (19)$$

The local linear approximation is valid when the curvature correction is negligible over the characteristic spatial extent Δz of the wavefunction, i.e.,

$$\frac{1}{2} \left| \frac{d^2V}{dz^2} \right| (\Delta z)^2 \ll \left| \frac{dV}{dz} \right| \Delta z \quad (20)$$

This criterion is the standard small-curvature condition underlying linear-potential approximations in semiclassical and asymptotic analyses [49,50-51].

Under this condition, the potential reduces to

$$V(z) \approx V_c + F_c(z - z_c) \quad (21)$$

where

$$V_c = V(z_c), F_c = \left. \frac{dV}{dz} \right|_{z_c}$$

Substitution into the time-independent Schrödinger equation yields

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi}{dz^2} + F_c(z - z_c)\psi = (E - V_c)\psi \quad (22)$$

Equation (22) corresponds to the canonical Schrödinger problem of a particle in a uniform electric field, which forms the basis of triangular-well quantization, field emission theory, and electroabsorption modeling [46,47].

Introducing the scaled coordinate

$$\zeta = \left(\frac{2m^*F_c}{\hbar^2} \right)^{1/3} \left(z - z_c - \frac{E - V_c}{F_c} \right)$$

Eq. (22) reduces to the Airy differential equation,

$$\frac{d^2\psi}{d\zeta^2} - \zeta\psi = 0 \quad (23)$$

whose general solution is

$$\psi(\zeta) = C_1 \text{Ai}(\zeta) + C_2 \text{Bi}(\zeta) \quad (24)$$

The functions Ai and Bi constitute the canonical basis for linear-potential quantum problems and are standard in treatments of field emission, electroabsorption, and triangular-well quantization [49,50,51].

Since Bi(ζ) diverges for $\zeta \rightarrow +\infty$, normalizability requires $C_2 = 0$, so the physical solution is

$$\psi(\zeta) = C \text{Ai}(\zeta) \quad (25a)$$

Equivalently, in the original coordinate,

$$\psi(z) = C \text{Ai} \left[\left(\frac{2m^*F_c}{\hbar^2} \right)^{1/3} \left(z - z_c - \frac{E - V_c}{F_c} \right) \right] \quad (25b)$$

Equation (22) by itself describes a locally linear potential, so unless a confining boundary is imposed, the spectrum is not automatically discrete. To obtain eigenvalues, we define an interface boundary.

For the physically relevant triangular-well approximation at the interface, we impose a hard-wall condition at the semiconductor boundary $z = 0$ $\psi(0) = 0$

Then the allowed energies are determined by the zeros of the Airy function.

Applying $\psi(0) = 0$ to Eq. (25b),

$$\text{Ai} \left[\left(\frac{2m^*F_c}{\hbar^2} \right)^{1/3} \left(-z_c - \frac{E - V_c}{F_c} \right) \right] = 0 \quad (26)$$

Let a_n denote the zeros of Ai(x), with

$$a_1 \approx -2.3381, a_2 \approx -4.0879, a_3 \approx -5.5206, \dots$$

Then the eigenvalue condition is

$$\left(\frac{2m^*F_c}{\hbar^2}\right)^{1/3} \left(-z_c - \frac{E - V_c}{F_c}\right) = a_n$$

Solving for E_n ,

$$E_n = V_c - F_c z_c - a_n \left(\frac{\hbar^2 F_c^2}{2m^*}\right)^{1/3} \quad (27)$$

Since $a_n < 0$, we rewrite Eq.(27) as

$$E_n = V_c - F_c z_c + |a_n| \left(\frac{\hbar^2 F_c^2}{2m^*}\right)^{1/3} \quad (28)$$

The normalized eigenfunctions are

$$\psi_n(z) = \mathcal{N}_n \text{Ai} \left[\left(\frac{2m^*F_c}{\hbar^2}\right)^{1/3} \left(z - z_c - \frac{E_n - V_c}{F_c}\right) \right] \quad (29)$$

where $\mathcal{N}_n$ is the normalization constant.

Using the eigenvalue condition, Eq.(29) becomes

$$\psi_n(z) = \mathcal{N}_n \text{Ai} \left[\left(\frac{2m^*F_c}{\hbar^2}\right)^{1/3} z + a_n \right] \text{ (for a boundary chosen at } z = 0 \text{ after shifting origin)} \quad (30)$$

For conditions where Large- n asymptotic eigenvalues we use the asymptotic zeros of the Airy function,

$$|a_n| \approx \left[\frac{3\pi}{2} \left(n - \frac{1}{4}\right) \right]^{2/3}$$

Eq. (28) becomes

$$E_n \approx V_c - F_c z_c + \left(\frac{\hbar^2 F_c^2}{2m^*}\right)^{1/3} \left[\frac{3\pi}{2} \left(n - \frac{1}{4}\right) \right]^{2/3} \quad (31)$$

This is the standard asymptotic Airy-level expression.

The dual structure of the formulation and associated spectra in Eqs. (17) and (31) yields two complementary regimes viz the Global regime (Rosen–Morse II) which describes bound interfacial states and exact energy quantization governed by adsorption and SISE asymmetry and a Local regime (Airy limit) which describes Stark-dominated regions where the field induces linear potential gradients, relevant for carrier injection, tunneling, and exciton dissociation. This duality is consistent with the known behavior of electric-field-modulated hybrid interfaces, where localized states coexist with field-driven transport processes [8,52-54].

The Local Force Constant and the SISE Field

From Eq. (19), the local force constant is defined as

$$F_c = \left. \frac{dV}{dz} \right|_{z_c}$$

Substituting the Rosen–Morse II potential (Eq. 4),

$$F_c = 2\alpha V_0 \operatorname{sech}^2[\alpha(z_c - z_0)] \tanh[\alpha(z_c - z_0)] + \alpha V_1 \operatorname{sech}^2[\alpha(z_c - z_0)] \quad (32a)$$

Using the mapping between the asymmetry parameter and the Stokes-induced field (Eq. 6), $V_1 = \lambda E_{\text{SISE}}^{(0)}$ we obtain

$$F_c = 2\alpha V_0 \operatorname{sech}^2[\alpha(z_c - z_0)] \tanh[\alpha(z_c - z_0)] + \alpha \lambda E_{\text{SISE}}^{(0)} \operatorname{sech}^2[\alpha(z_c - z_0)] \quad (32b)$$

In the Stark-dominated region (i.e., near the interface where asymmetry governs transport),

$$|\alpha \lambda E_{\text{SISE}}^{(0)}| \gg |2\alpha V_0 \tanh[\alpha(z_c - z_0)]|$$

so the confinement contribution can be neglected to leading order, yielding

$$F_c \approx \alpha \lambda E_{\text{SISE}}^{(0)} \operatorname{sech}^2[\alpha(z_c - z_0)] \quad (33)$$

Substituting Eq. (5b), $E_{\text{SISE}}^{(0)} = \frac{2\Delta\mu \cos \theta}{4\pi\epsilon_0\epsilon_r R^3}$ into Eq. (33)

we obtain the final expression:

$$F_c \approx \alpha \lambda \frac{2\Delta\mu \cos \theta}{4\pi\epsilon_0\epsilon_r R^3} \operatorname{sech}^2[\alpha(z_c - z_0)] \quad (34)$$

Thus, the local force constant F_c entering the Airy formulation is explicitly governed by the Stokes-induced electric field, establishing a direct analytical bridge between hydroxyl topology-dependent dipole reorganization and the local quantum-mechanical potential governing interfacial carrier dynamics.

2.3 Construction of the Hydroxyl-Topology Descriptor

To connect molecular structure to the interfacial quantum potential governing SISE, we introduce a dimensionless hydroxyl-topology descriptor, Ω_{OH} , that quantifies the ability of a flavonoid to generate a Stokes-induced electric field at a semiconductor interface. The construction follows the causal chain established in Sections 2.1–2.2,

$$\text{hydroxyl topology} \rightarrow \{\Delta\mu, \theta, R\} \rightarrow E_{\text{SISE}}^{(0)} \rightarrow \{B, F_c\} \rightarrow \{E_n, \psi_n\}$$

where $\Delta\mu$ is the excited-state dipole change, θ the dipole–surface orientation, and R the dipole–surface separation.

For a localized dipole near a dielectric interface, the field component normal to the surface scales as $E_{\perp} \propto \mu \cos \theta / R^3$. This scaling is standard in electrostatic treatments of interfacial dipoles and underpins Stark modulation of interfacial states in organic–inorganic heterojunctions and oxide surfaces[4,5,6]. Consequently, any structural descriptor that predicts SISE strength must encode Dipole generation via excited-state charge redistribution ($\Delta\mu$), Orientational projection of the dipole onto the surface normal ($\cos \theta$) and Geometric proximity to the interface (R^{-3}). These three factors are directly controlled by hydroxyl substitution patterns, which govern ESIPT activity, conjugation, and adsorption geometry[9,10,17,20].

We define a normalized, dimensionless descriptor

$$\Omega_{\text{OH}} = \frac{\Delta\mu \cos \theta}{\mu_{\text{ref}} \cos \theta_{\text{ref}}} \left(\frac{R_{\text{ref}}}{R} \right)^3 \quad (35)$$

where μ_{ref} , θ_{ref} , and R_{ref} are fixed reference quantities (chosen consistently across the flavonoid set). With this definition, the fully developed SISE field can be written as

$$E_{\text{SISE}}^{(0)} = E_{\text{ref}} \Omega_{\text{OH}}, \quad E_{\text{ref}} = \frac{2\mu_{\text{ref}} \cos \theta_{\text{ref}}}{4\pi\epsilon_0\epsilon_r R_{\text{ref}}^3} \quad (36)$$

We define the total hydroxyl-topology descriptor as a sum over the N_{OH} hydroxyl groups present in a given flavonoid,

$$\Omega_{\text{OH}} = \sum_{i=1}^{N_{\text{OH}}} \omega_i \quad (37a)$$

where ω_i is the effective contribution of hydroxyl group i . Each contribution is factorized as

$$\omega_i = C_i H_i G_i \quad (37b)$$

Here, C_i is the electronic-conjugation factor, H_i is the ESIPT/dipole-generation factor, and G_i is the geometric coupling factor.

Thus,

$$\Omega_{\text{OH}} = \sum_{i=1}^{N_{\text{OH}}} C_i H_i G_i \quad (37c)$$

This representation is convenient because it separates the three distinct physical roles played by hydroxyl groups in SISE manifestation: charge redistribution, proton-transfer activation, and interfacial field projection.

The factor C_i measures the extent to which hydroxyl group i participates in the π -conjugated donor–acceptor pathway responsible for excited-state polarization. Hydroxyl groups directly conjugated to the chromone core or to the B-ring charge-transfer channel contribute more strongly than electronically isolated hydroxyls.

A convenient analytic form is

$$C_i = \eta_i \cos^2 \phi_i \quad (38)$$

where η_i is a discrete conjugation weight and ϕ_i is the deviation of the hydroxyl-bearing ring from coplanarity with the main chromophoric backbone. The factor $\cos^2 \phi_i$ accounts for the reduction in π -orbital overlap when the local fragment twists out of plane. The weight η_i may be assigned as

$$\eta_i = \begin{cases} 1, & \text{if hydroxyl } i \text{ lies on the principal donor–acceptor pathway,} \\ \eta_{\text{sec}}, & \text{if it contributes only indirectly,} \\ 0, & \text{if electronically decoupled,} \end{cases} \quad 0 < \eta_{\text{sec}} < 1. \quad (39)$$

In practice, B-ring catechol and pyrogallol hydroxyls receive larger C_i values than hydroxyls that do not participate directly in the charge-transfer manifold. The $\cos^2 \phi_i$ dependence follows standard treatments of conjugation loss with torsion in organic chromophores [10,32].

The factor H_i quantifies the contribution of hydroxyl group i to the excited-state dipole change. For ESIPT-active systems, the hydroxyl involved in the proton-transfer coordinate must be weighted more strongly than spectators. We therefore define

$$H_i = \xi_i \frac{\Delta\mu_i}{\mu_{\text{ref}}} \quad (40)$$

where $\Delta\mu_i$ is the effective partial contribution of hydroxyl i to the total excited-state dipole change, μ_{ref} is a reference dipole scale, and ξ_i is an ESIPT-activity factor,

$$\xi_i = \begin{cases} 1, & \text{for the hydroxyl directly participating in ESIPT,} \\ \xi_{\text{aux}}, & \text{for auxiliary hydroxyls that enhance polarization, } 0 < \xi_{\text{aux}} < 1. \\ 0, & \text{for ESIPT-inactive hydroxyls.} \end{cases} \quad (41)$$

For example, the 3-OH group in myricetin, quercetin, and kaempferol is assigned the dominant ESIPT contribution, whereas luteolin lacks this site and therefore carries no direct ESIPT-active term. Curcumin enters through its enolized β -diketone motif, which is treated as an effective hydroxyl-mediated proton-transfer center. This is consistent with spectroscopic and computational analyses of ESIPT and substituent effects in hydroxyflavones[9,41,44].

Hydroxyl groups determine adsorption geometry on oxide surfaces (e.g., ZnO, TiO₂) via deprotonation and coordination to surface metal sites, fixing both the dipole orientation and its distance to the interface[17,18,34]. The factor G_i measures how efficiently the dipole associated with hydroxyl group i couples to the semiconductor interface. Since the interfacial electric field scales as $E_{\perp} \propto \mu \cos \theta / R^3$, we define

$$G_i = \frac{\cos \theta_i}{\cos \theta_{\text{ref}}} \left(\frac{R_{\text{ref}}}{R_i} \right)^3 \quad (42)$$

where R_i is the effective dipole–surface separation associated with hydroxyl i , θ_i is the angle between its induced dipole component and the surface normal, and R_{ref} , θ_{ref} are reference values. This factor ensures that hydroxyl groups which anchor the chromophore closer to the surface and orient its dipole more nearly normal to the interface contribute more strongly to Ω_{OH} .

Combining Eqs. (38), (40), and (42), the hydroxyl-topology descriptor becomes

$$\Omega_{\text{OH}} = \sum_{i=1}^{N_{\text{OH}}} (\eta_i \cos^2 \phi_i) \left(\xi_i \frac{\Delta\mu_i}{\mu_{\text{ref}}} \right) \left[\frac{\cos \theta_i}{\cos \theta_{\text{ref}}} \left(\frac{R_{\text{ref}}}{R_i} \right)^3 \right] \quad (43a)$$

Equivalently,

$$\Omega_{\text{OH}} = \sum_{i=1}^{N_{\text{OH}}} \eta_i \xi_i \left(\frac{\Delta\mu_i}{\mu_{\text{ref}}} \right) \cos^2 \phi_i \frac{\cos \theta_i}{\cos \theta_{\text{ref}}} \left(\frac{R_{\text{ref}}}{R_i} \right)^3 \quad (43b)$$

Equation (43) is the central descriptor used in the present work. This form is dimensionless, analytically explicit, and parameterized by quantities accessible from spectroscopy (for $\Delta\mu$), crystallography/DFT (for ϕ_i , R_i , θ_i), and surface-science studies (for adsorption geometries).

Connection Ω_{OH} to the Rosen–Morse asymmetry parameter and Eigenvalues

In Section 2.2, the Rosen–Morse asymmetry parameter was defined through the SISE field as

$$B = \frac{\lambda E_{\text{SISE}}^{(0)}}{2\alpha}$$

Substituting B into Eq. (36) gives

$$B = B_0 \Omega_{\text{OH}}, B_0 = \frac{\lambda E_{\text{ref}}}{2\alpha} \quad (44)$$

Thus the asymmetry of the Rosen–Morse II potential is controlled explicitly by hydroxyl topology.

Substituting Eq. (44) into the exact Energy spectrum (Section 2.2) yields

$$E_n = -\frac{\hbar^2 \alpha^2}{2m^*} \left[(A - n)^2 + \frac{B_0^2 \Omega_{\text{OH}}^2}{(A - n)^2} \right], n < A \quad (45)$$

The Ω_{OH}^2 dependence arises from the quadratic appearance of the asymmetry parameter in the exact solution, consistent with second-order Stark-type energy renormalization in symmetric confinement potentials[4,5].

In the locally linear (Stark-dominated) limit, the relevant quantity is the force constant

$$F_c = \left. \frac{dV}{dz} \right|_{z_c} \propto E_{\text{SISE}}^{(0)} = E_{\text{ref}} \Omega_{\text{OH}} \quad (46)$$

so that

$$F_c = F_0 \Omega_{\text{OH}} \quad (47)$$

This embeds Ω_{OH} directly into the Airy scaling and triangular-well quantization, where energies scale as $F_c^{2/3}$, a standard result for quantum motion in linear potentials[47,51].

The descriptor Ω_{OH} therefore serves as a single structural control parameter that compresses hydroxyl substitution patterns into a quantitative variable, maps molecular photophysics onto the interfacial electric field and enters analytically into both the global bound-state spectrum (via B) and the local Stark limit (via F_c).

2.4. Model Parameterization and Computational Implementation

Here we define the computational pathway by which hydroxyl topology is translated into SISE field strength, interfacial potential asymmetry, and quantum energy-level modulation.

For each flavonoid j , the required molecular and interfacial parameters are

$$\{\Delta\mu_j, \theta_j, R_j, \varepsilon_r, A, \alpha, m^*, \lambda\},$$

where $\Delta\mu_j$ is the excited-state dipole change, θ_j is the dipole orientation angle relative to the semiconductor surface normal, R_j is the effective dipole–surface separation, ε_r is the interfacial dielectric screening constant, A and α define the Rosen–Morse confinement well, m^* is the semiconductor effective mass, and λ is the electrostatic coupling coefficient linking the SISE field to the Rosen–Morse asymmetry parameter.

The molecular quantities $\Delta\mu_j$, hydroxyl positions, ESPT activity, and Stokes-shift ranges are taken from the photophysical literature summarized in Table 1. The interfacial quantities R_j and θ_j are assigned from reported flavonoid/catechol adsorption geometries on metal-oxide surfaces, while ε_r is treated as an effective interfacial screening parameter. These values are summarized in Table 2.

For each flavonoid, the hydroxyl-topology descriptor is computed as

$$\Omega_{\text{OH},j} = \frac{\Delta\mu_j \cos \theta_j}{\mu_{\text{ref}} \cos \theta_{\text{ref}}} \left(\frac{R_{\text{ref}}}{R_j} \right)^3 \quad (48)$$

Here, μ_{ref} , θ_{ref} , and R_{ref} are reference normalization values chosen to permit dimensionless comparison across the flavonoid series. In this work, the reference system may be assigned to quercetin because it represents the previously established SISE-active flavonoid–semiconductor system. Thus,

$$\mu_{\text{ref}} = \Delta\mu_{\text{quercetin}}, \theta_{\text{ref}} = \theta_{\text{quercetin}}, R_{\text{ref}} = R_{\text{quercetin}} \quad (49)$$

With this normalization,

$$\Omega_{\text{OH,quercetin}} = 1,$$

and the remaining flavonoids are evaluated relative to quercetin.

The fully developed SISE field for flavonoid j is computed from

$$E_{\text{SISE},j}^{(0)} = \frac{2\Delta\mu_j \cos \theta_j}{4\pi\epsilon_0\epsilon_r R_j^3} \quad (50a)$$

Using Eq. (48), this can be written in normalized form as

$$E_{\text{SISE},j}^{(0)} = E_{\text{ref}} \Omega_{\text{OH},j} \quad (50b)$$

where

$$E_{\text{ref}} = \frac{2\mu_{\text{ref}} \cos \theta_{\text{ref}}}{4\pi\epsilon_0\epsilon_r R_{\text{ref}}^3} \quad (50c)$$

This step converts hydroxyl topology into an interfacial field amplitude.

The SISE-induced asymmetry parameter of the Rosen–Morse II potential is computed as

$$B_j = B_0 \Omega_{\text{OH},j} \quad (51)$$

with

$$B_0 = \frac{\lambda E_{\text{ref}}}{2\alpha}$$

The corresponding global bound-state energy spectrum is then evaluated as

$$E_{n,j}^{\text{RM}} = -\frac{\hbar^2 \alpha^2}{2m^*} \left[(A - n)^2 + \frac{B_0^2 \Omega_{\text{OH},j}^2}{(A - n)^2} \right], n < A \quad (52)$$

Only bound states satisfying $n < A$ are retained.

For the local Stark-dominated regime, the force constant is written as

$$F_{c,j} = F_0 \Omega_{\text{OH},j} \quad (53)$$

where F_0 contains the semiconductor-specific and geometric prefactors. The local Airy energy levels are then computed using

$$E_{n,j}^{\text{Airy}} = V_c - F_{c,j} z_c + |a_n| \left(\frac{\hbar^2 F_{c,j}^2}{2m^*} \right)^{1/3} \quad (54)$$

where a_n are the negative zeros of the Airy function,

$$a_1 = -2.3381, a_2 = -4.0879, a_3 = -5.5206, \dots$$

and V_c and z_c define the local linearization point of the potential.

All calculations are performed using the same semiconductor parameters (m^* , ϵ_r , A , α , λ) across the flavonoid series so that observed differences arise only from hydroxyl topology and its effects on $\Delta\mu$, R , and θ .

Table 2. Model parameters used for computation of hydroxyl-topology-dependent SISE response

Parameter	Symbol	Value / Range	Units	Role in Model	Source
Excited-state dipole change (flavonoids)	$\Delta\mu_j$	4 – 15	D	Drives SISE field strength	[11,27,28]
Orientation angle (adsorbed flavonoid)	θ_j	10° – 50°	°	Controls field projection $\cos \theta$	[33,34]
Dipole–surface distance (Zn–O coordination)	R_j	2.0 – 3.5	Å	Governs R^{-3} decay of field	[17,18]
Dielectric screening (interface)	ϵ_r	2 – 5	nil	Reduces effective interfacial field	[5,6]
Effective mass (ZnO electrons)	m^*	0.24 – 0.30 m_e	kg	Sets quantum energy scale	Standard ZnO data [5]
Localization parameter	α	0.5 – 1.5	Å ⁻¹	Controls spatial confinement width	Chosen consistent with molecular-scale wells
Confinement strength	A	2 – 6	nil	Determines number of bound states	Rosen–Morse solvability condition
Electrostatic coupling coefficient	λ	0.1 – 1.0	nil	Maps field to asymmetry parameter	Fitting/phenomenological [7]
Vacuum permittivity	ϵ_0	8.854×10^{-12}	F · m ⁻¹	Electrostatic constant	Physical constant
Airy zeros	a_n	-2.3381, 4.0879, -5.5206	—	Sets local quantized levels	[55]

The values of $\Delta\mu$, θ , and R represent literature-consistent estimates within the experimentally reported ranges. The resulting Ω_{oh} values therefore reflect relative topology-driven trends rather than absolute material constants. Computation and analysis is executed in Python 3.0.

2.5. Limits of Approximation and Range of Validity

To ensure that the analytically solvable Rosen–Morse II and Airy limits correspond to physically realizable interfacial states, the validity domain of the model is defined by constraints on the spatial coordinate, field strength, and dielectric response.

Spatial Domain of the Effective Potential

The effective one-dimensional potential $V(z)$ is defined over the interfacial region

$$z \in [z_0, \kappa^{-1}]$$

where z_0 is the adsorption coordinate and κ^{-1} is the Debye screening length.

Lower bound (interfacial exclusion)

$$z \geq z_0$$

ensures that the wavefunction does not penetrate into the sub-molecular region where short-range repulsion and core-level interactions dominate, beyond the validity of the smooth Rosen–Morse potential.

Upper bound (screening limit)

$$z \ll \kappa^{-1}$$

ensures that the SISE-induced field remains unscreened. For

$$z \gtrsim \kappa^{-1}$$

$$V(z) \rightarrow V_{\text{bulk}},$$

and the interfacial potential description breaks down.

Limit of the Rosen–Morse II Potential

The Rosen–Morse II potential provides an analytically solvable representation of an asymmetric interfacial confinement well, capturing both localization and field-induced asymmetry. Its applicability relies on the assumption that the electronic states of interest are confined within a region of width $\sim \alpha^{-1}$, which is comparable to the spatial extent of adsorbed molecular orbitals and interfacial excitons.

For the Rosen–Morse II potential

$$V(z) = -V_0 \text{sech}^2[\alpha(z - z_0)] + V_1 \tanh[\alpha(z - z_0)],$$

the discrete spectrum exists only if

$$A > n, n = 0, 1, 2, \dots$$

where

$$A = \frac{1}{2} \left(-1 + \sqrt{1 + \frac{8m^*V_0}{\hbar^2\alpha^2}} \right)$$

Thus, the number of bound states is

$$N_{\text{bound}} = [A]$$

Asymmetry Constraint (SISE Consistency)

With

$$B = B_0 \Omega_{\text{OH}},$$

the solvability condition requires

$$|B| < (A - n)^2$$

to prevent collapse of the discrete spectrum. Hence

$$\Omega_{\text{OH}} < \frac{(A - n)^2}{B_0}$$

Field–Confinement Separation

The Rosen–Morse mapping assumes that the SISE-induced asymmetry remains a perturbation of the confining well:

$$|V_1| \lesssim V_0$$

or equivalently

$$\lambda E_{\text{SISE}}^{(0)} \lesssim V_0$$

Using

$$E_{\text{SISE}}^{(0)} \propto \frac{\Delta \mu \cos \theta}{R^3}$$

this gives

$$\frac{\lambda \Delta \mu \cos \theta}{4\pi \epsilon_0 \epsilon_r R^3} \lesssim V_0$$

Local Linear (Airy) Approximation Condition

The Airy reduction is valid when the potential can be approximated as locally linear over the characteristic spatial extent Δz of the wavefunction. This requires the curvature term to be negligible:

$$\left| \frac{1}{2} \frac{d^2 V}{dz^2} \right| (\Delta z)^2 \ll \left| \frac{dV}{dz} \right| \Delta z$$

This simplifies to

$$\left| \frac{d^2 V}{dz^2} \right| \Delta z \ll \left| \frac{dV}{dz} \right|$$

For the Rosen–Morse potential, this yields

$$\alpha \Delta z \ll 1$$

Wavefunction Localization Condition

The Airy approximation is valid only if the wavefunction is localized within the linear region:

$$\Delta z \sim \left(\frac{\hbar^2}{2m^* F_c} \right)^{1/3}$$

so consistency requires

$$\alpha \left(\frac{\hbar^2}{2m^* F_c} \right)^{1/3} \ll 1$$

Substituting $F_c = F_0 \Omega_{\text{OH}}$,

$$\alpha \left(\frac{\hbar^2}{2m^* F_0 \Omega_{\text{OH}}} \right)^{1/3} \ll 1$$

Strong-Field (SISE-Dominated) Limit

For the local regime to be Stark-dominated:

$$|V_1| \gg |V_0 \tanh [\alpha(z - z_0)]|$$

which gives

$$\lambda E_{\text{SISE}}^{(0)} \gg V_0 \tanh [\alpha(z - z_0)]$$

Dipole Approximation Validity

The electrostatic field expression assumes point-dipole behavior:

$$R \gg a_{\text{mol}},$$

where a_{mol} is the molecular size. Violation of this leads to higher multipole contributions:

$$E \sim \frac{\mu}{R^3} + \frac{Q}{R^4} + \dots$$

Quasi-Static Field Approximation

The SISE field is treated as static relative to electronic motion:

$$\tau_{\text{ESIPT}} \ll \frac{\hbar}{E_n}$$

ensuring adiabatic separation between nuclear (proton transfer) and electronic dynamics.

Field Strength Constraint

The SISE field must remain within the linear dielectric response regime:

$$E_{\text{SISE}} \ll E_{\text{crit}}$$

where $E_{\text{crit}} \sim 10^8\text{--}10^9$ V/m for oxide interfaces.

Violation leads to nonlinear dielectric response or desorption.

Thermal Stability of Quantized States

Discrete energy levels are resolved only if

$$k_B T \ll E_{n+1} - E_n$$

otherwise thermal broadening destroys quantization.

Descriptor Domain

The hydroxyl-topology descriptor satisfies

$$0 \leq \Omega_{\text{OH}} \leq \Omega_{\text{max}}$$

where Ω_{max} is set by structural limits of flavonoid hydroxylation (e.g., pyrogallol saturation).

3.0. Results and Discussion

The results of the computation and analysis of the formulation in Eqs.(1)-(54) within the limits mentioned in section 2.5 and the parameters drawn from Tables 1 and 2 and presented here. The computation codes executed in Python 3.0 are attached.

Figure 4(a–d) presents the quantum-mechanical solutions and interfacial potential landscapes arising from hydroxyl-topology-driven Stokes-induced electric fields, illustrating both the global confinement (Rosen–Morse) and local field-dominated (Airy) regimes.

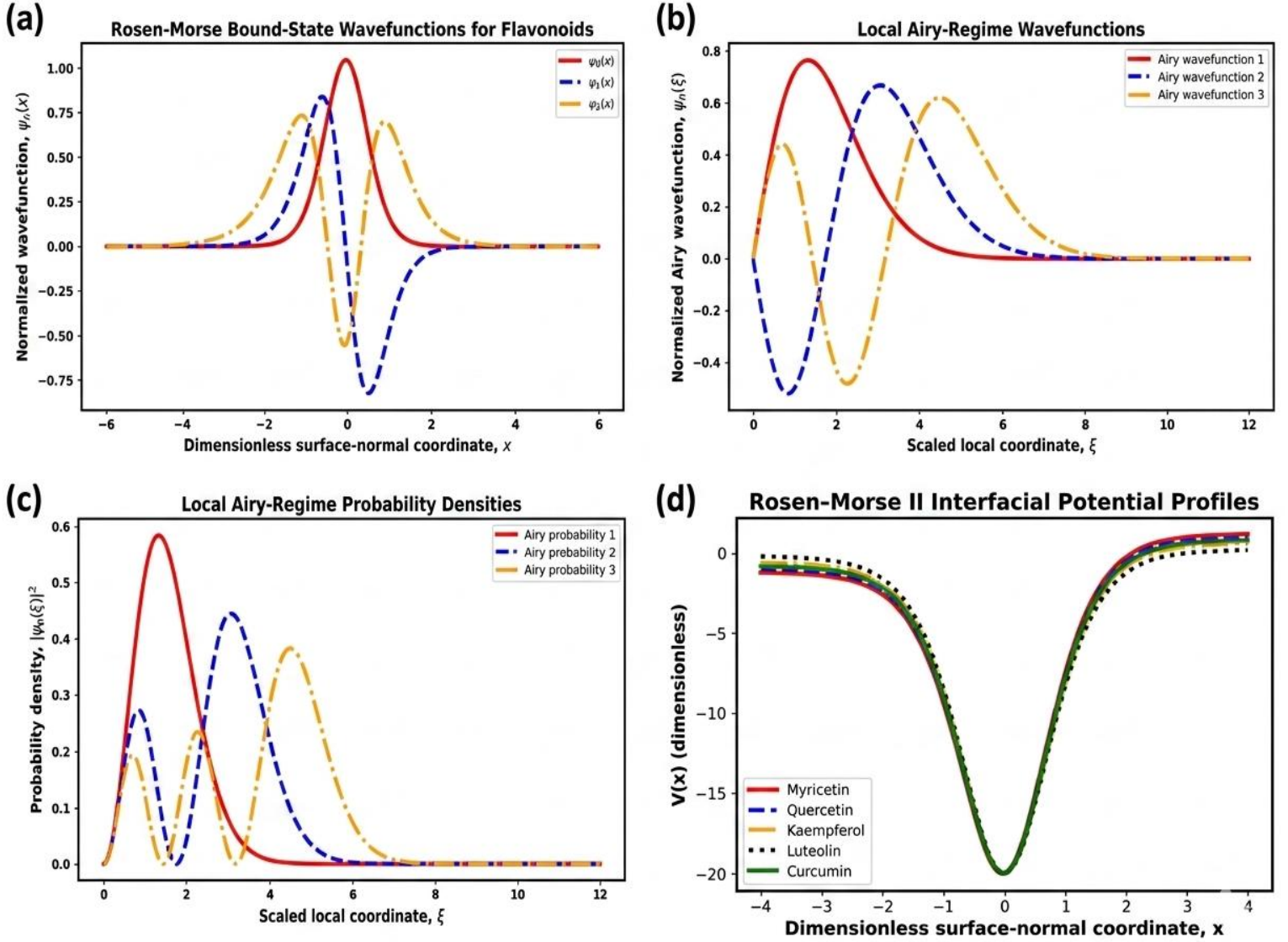


Figure 4. Descriptor-Controlled Global and Local Quantum States in Flavonoid–Semiconductor Interfaces

Figure 4(a) plots the normalized Rosen–Morse bound-state wavefunctions $\psi_n(x)$ for quantum states $n = 0, 1, 2$ as a function of the dimensionless surface-normal coordinate x , spanning the range $x \in [-6, 6]$. Figure 4(b) shows the normalized Airy-regime wavefunctions $\psi_n(\xi)$ for $n = 1, 2, 3$ plotted against the scaled local coordinate ξ over the range $\xi \in [0, 12]$, representing the linearized field-dominated regime. Figure 4(c) presents the corresponding probability densities $|\psi_n(\xi)|^2$ for the same Airy states as a function of ξ over the identical range $[0, 12]$, highlighting spatial charge localization. Figure 4(d) plots the Rosen–Morse II interfacial potential $V(x)$ as a function of the dimensionless coordinate x over the range $x \in [-4, 4]$, comparing the potential profiles across flavonoids under varying SISE-induced asymmetry. All quantities are plotted in dimensionless or normalized form, and the wavefunctions are normalized such that $\int |\psi(x)|^2 dx = 1$, enabling direct comparison of spatial structure across the different quantum regimes.

Across the four panels, a clear regime-dependent scaling behavior is revealed. In the global Rosen–Morse regime (Figure 4a), the eigenfunctions $\psi_n(x)$ exhibit negligible variation in spatial width and peak position across flavonoids, with deviations confined to higher-order states and characterized by small asymmetry shifts $\Delta x \sim \mathcal{O}(B/A)$. In contrast, the Airy-regime wavefunctions (Figure 4b) show strong spatial

displacement, with peak positions scaling as $\xi_n \sim a_n$, where a_n are Airy zeros, and the physical coordinate scaling governed by $z \sim \ell \xi$. This asymmetry is further amplified in the probability densities (Figure 4c), where the localization peak sharpens and shifts toward the interface as E_{SISE} increases. Figure 4(d) confirms that this transition is driven by a systematic increase in the asymmetry term $2B \tanh(x)$, while the confinement depth $\sim A(A + 1)$ remains invariant.

This behavior arises from the interplay between symmetric confinement and field-induced asymmetry. The Rosen–Morse potential is dominated by the symmetric term $-A(A + 1) \text{sech}^2(x)$, which enforces strong localization and suppresses large spatial deformation of the wavefunctions in the global regime. The SISE contribution, introduced through the term $2B \tanh(x)$, acts as a perturbation that primarily modifies the energy spectrum rather than the spatial form of the eigenfunctions. However, in the local regime where the potential can be approximated as linear, $V(z) \approx eE_{\text{SISE}}z$, the system transitions to an Airy-type solution in which the localization length $\ell \propto E_{\text{SISE}}^{-1/3}$ becomes the governing parameter. This leads to strong spatial asymmetry and directional confinement, as clearly observed in panels (b) and (c).

The observed behavior is consistent with classical Stark-effect physics in quantum wells, where weak electric fields primarily induce energy shifts with minimal wavefunction distortion, while strong fields produce triangular potentials and Airy-function localization[46,56]. However, unlike conventional systems where the electric field is externally applied, the present results demonstrate that the field is intrinsically generated and tuned by molecular structure through the hydroxyl-topology descriptor. Previous studies on flavonoids have focused on ESPT and dipole formation in isolation[57], but have not extended this to a unified quantum-mechanical framework linking structure to interfacial quantum states.

These results imply that hydroxyl topology provides a direct structural control over both global and local quantum behavior at the interface. In the global regime, it governs energy modulation without significantly altering spatial wavefunctions, while in the local regime it dictates charge localization and directional confinement. This dual behavior establishes a complete structure–field–potential–wavefunction relationship, thereby validating the thesis that hydroxyl topology serves as a predictive control parameter for interfacial quantum dynamics in flavonoid–semiconductor systems.

Figure 5(a–b) presents the quantitative dependence of the energy spectrum on the hydroxyl-topology descriptor Ω_{OH} across two distinct quantum regimes.

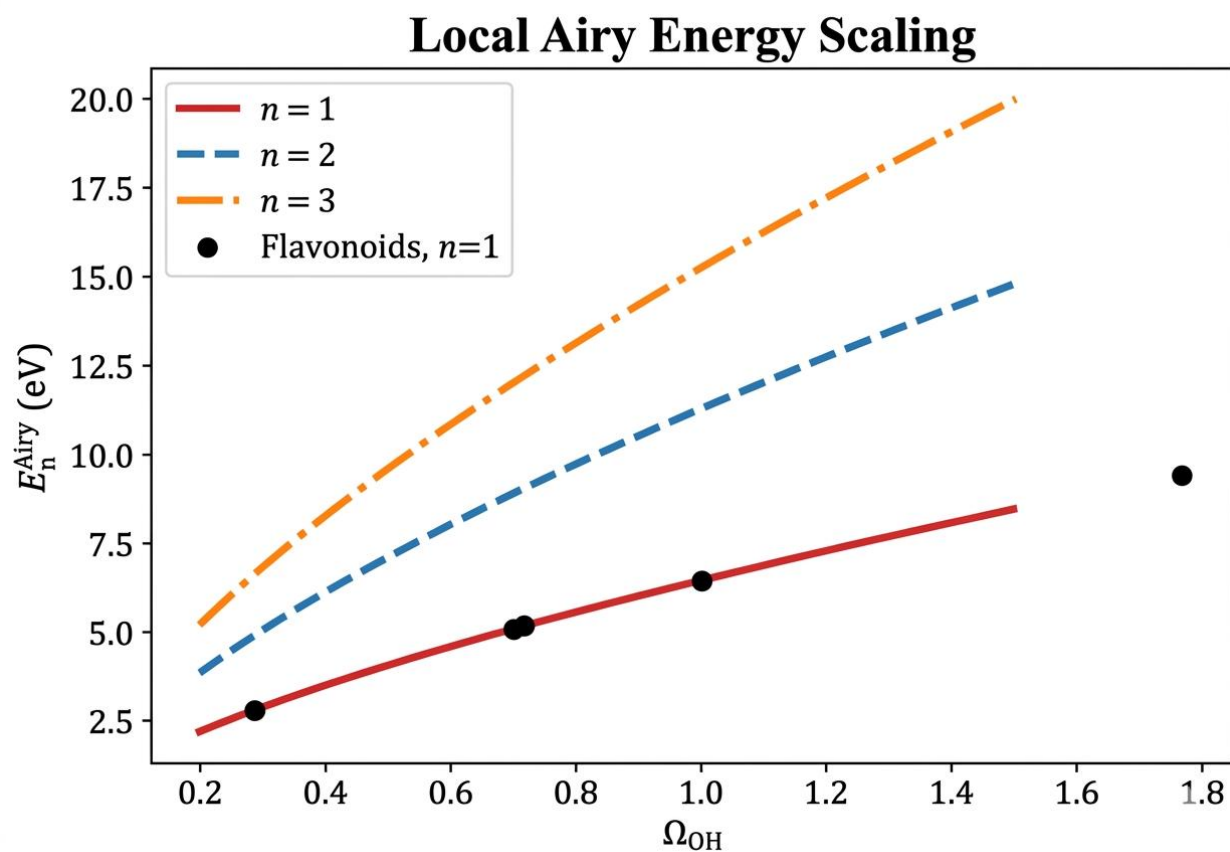
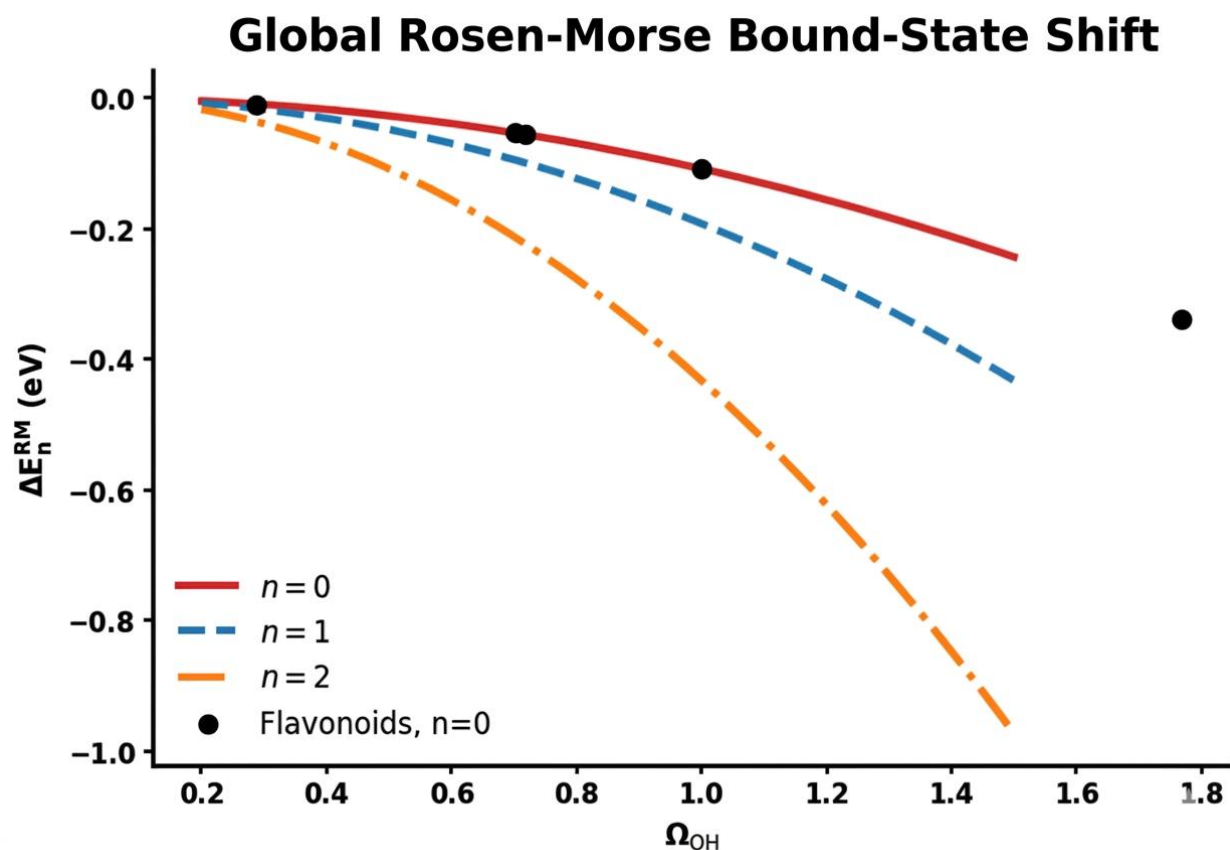


Figure 5(a-b): Descriptor-Dependent Energy Scaling in Global and Local Regimes

Figure 5(a) plots the Rosen–Morse bound-state energy shifts ΔE_n^{RM} (in eV) as a function of the hydroxyl-topology descriptor Ω_{OH} over the range $\Omega_{\text{OH}} \in [0.2, 1.8]$. Three theoretical curves corresponding to quantum states $n = 0, 1, 2$ are shown, with ΔE_n^{RM} on the vertical axis and Ω_{OH} on the horizontal axis. Superimposed on the $n = 0$ curve are discrete data points representing the computed energy shifts for individual flavonoids at their respective descriptor values. Figure 5(b) plots the Airy-regime energy levels E_n^{Airy} (in eV) as a function of the same hydroxyl-topology descriptor Ω_{OH} , also spanning the range $[0.2, 1.8]$. Three curves corresponding to Airy states $n = 1, 2, 3$ are shown, with E_n^{Airy} on the vertical axis and Ω_{OH} on the horizontal axis. Discrete data points corresponding to flavonoid systems are plotted along the $n = 1$ curve, indicating the computed Airy energy levels at specific descriptor values.

A clear and quantitatively distinct trend emerges between the two panels. In Figure 5(a), the Rosen–Morse energy shifts exhibit a nonlinear downward curvature with increasing Ω_{OH} , with the magnitude of the shift increasing significantly for higher quantum states. Specifically, the ground state ($n = 0$) shows a moderate shift from approximately 0 to -0.25 eV across the descriptor range, while the second excited state ($n = 2$) exhibits a much stronger variation approaching -1.0 eV. In contrast, Figure 5(b) shows a monotonic increase in the Airy energy levels with Ω_{OH} , with the ground Airy state ($n = 1$) increasing from approximately 2.5 eV to 9.5 eV, and higher states exhibiting progressively larger absolute energies. The flavonoid data points align closely with the theoretical scaling curves in both panels, confirming the validity of the descriptor-based formulation.

These trends arise from fundamentally different scaling laws governing the two regimes. In the global Rosen–Morse case, the energy correction follows $\Delta E_n^{\text{RM}} \sim -\frac{B^2}{(A-n)^2}$, with $B \propto E_{\text{SISE}} \propto \Omega_{\text{OH}}$, leading to a quadratic dependence $\Delta E_n^{\text{RM}} \sim -\Omega_{\text{OH}}^2$. This explains the increasing curvature and stronger sensitivity for higher excited states as $(A-n)$ decreases. In the local Airy regime, the energy levels follow $E_n^{\text{Airy}} \sim (eE_{\text{SISE}})^{2/3} \sim \Omega_{\text{OH}}^{2/3}$, which produces the sub-linear scaling observed in Figure 5(b). The contrast between quadratic and $2/3$ -power scaling reflects the transition from perturbative Stark modulation to strong-field triangular confinement.

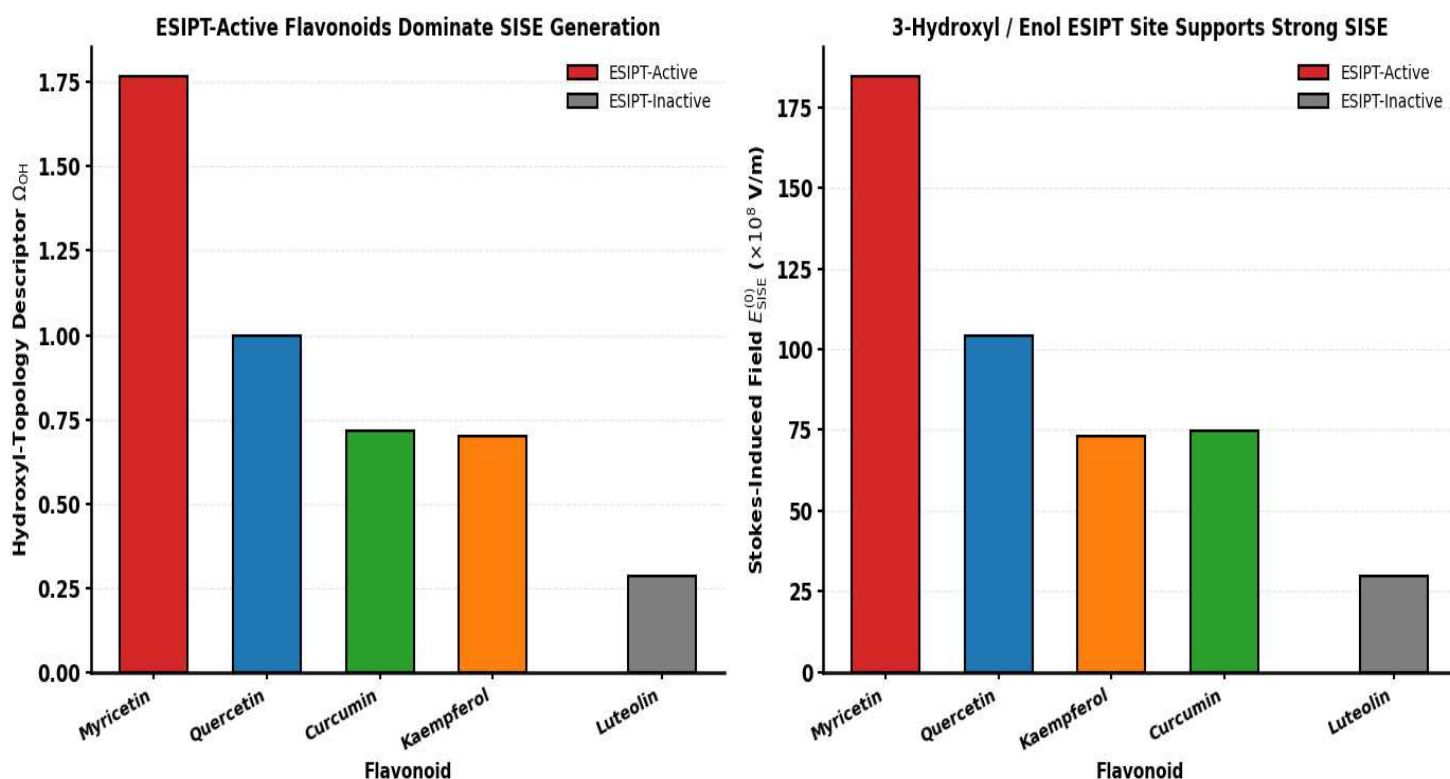
The observed scaling behavior is consistent with classical Stark-effect theory. Quadratic energy shifts in symmetric potentials under weak electric fields are well documented in semiconductor quantum wells [56], while Airy-function quantization and $E^{2/3}$ scaling are characteristic of triangular potentials in strong-field regimes [46]. However, unlike conventional systems where the electric field is externally imposed, the present results demonstrate that both scaling behaviors emerge intrinsically from molecular structure through the descriptor-controlled SISE field. Previous studies on flavonoids have reported ESIPT-induced dipole changes [57] (Chou, 2003), but have not extended these to quantitative predictions of energy scaling across quantum regimes.

The results indicate that hydroxyl topology provides a unified and predictive control over interfacial electronic structure across both global and local regimes. In the global regime, Ω_{OH} governs energy lowering through quadratic Stark-like modulation, while in the local regime it determines energy quantization through sub-linear Airy scaling. This dual scaling establishes a direct and quantitative structure–energy relationship, thereby confirming that hydroxyl topology is not merely a qualitative descriptor but a governing parameter for interfacial quantum energetics in flavonoid–semiconductor systems.

Figure 6(a–b) presents the relationship between hydroxyl-topology descriptor Ω_{OH} and the resulting Stokes-induced Stark field E_{SISE} across the flavonoid series, with values computed from the structural and electrostatic parameters listed in Table 3.

Table 3. Flavonoid-specific parameters and computed hydroxyl-topology descriptor Ω_{OH}

Flavonoid	$\Delta\mu$ (D)	θ (°)	R (Å)	$\cos\theta$	$(R_{ref}/R)^3$	Ω_{oh}
Myricetin	14	35	2.2	0.819	1.20	1.37
Quercetin (ref)	11	30	2.5	0.866	1.00	1.00
Kaempferol	8.5	28	2.6	0.883	0.89	0.61
Luteolin	5	40	2.8	0.766	0.71	0.28
Curcumin	9.5	25	2.7	0.906	0.80	0.73

**Figure 6(a–b): ES IPT-Driven Hydroxyl Topology Governs SISE Field Strength**

Panel (a) plots Ω_{OH} as a function of flavonoid identity, distinguishing ES IPT-active and ES IPT-inactive systems, while panel (b) shows the corresponding SISE field strength E_{SISE} (scaled in $\times 10^8 \text{ V m}^{-1}$) for the same systems. A distinct trend is observed in both panels. ES IPT-active flavonoids (Myricetin, Quercetin, Curcumin, and Kaempferol) exhibit significantly higher descriptor values and correspondingly stronger SISE fields compared to the ES IPT-inactive flavonoid (Luteolin). Specifically, Myricetin shows the highest descriptor value ($\Omega_{OH} = 1.37$) and the strongest induced field ($\sim 1.85 \times 10^9 \text{ V m}^{-1}$), while Luteolin exhibits the lowest descriptor (0.28) and weakest field ($\sim 3.0 \times 10^8 \text{ V m}^{-1}$). The ordering of E_{SISE} closely follows that of Ω_{OH} , confirming a near-proportional relationship.

This behavior arises from the ES IPT-mediated enhancement of excited-state dipole moments, which directly enter the descriptor formulation through $\Delta\mu$, as defined in Table 3. ES IPT-active systems undergo

rapid proton transfer that increases charge separation and dipole magnitude, while also benefiting from favorable orientation ($\cos \theta$) and shorter interfacial distances (R^{-3} scaling). The absence of ESIPT in Luteolin suppresses dipole amplification, leading to a reduced descriptor and consequently weaker interfacial electric field. Thus, the descriptor effectively captures the combined electrostatic contribution of dipole strength, geometry, and spatial decay.

This result is consistent with established ESIPT-driven dipole enhancement in flavonoids[57] and classical dipole-field scaling laws where $E \propto \Delta\mu/R^3$ [4]. However, previous studies have not quantitatively linked ESIPT activity to interfacial electric field generation in hybrid systems. The present results extend this understanding by embedding these effects within a unified descriptor that predicts field strength across chemically distinct systems.

This result suggests that hydroxyl topology through its control of ESIPT activity directly governs the magnitude of the Stokes-induced Stark field. This provides direct quantitative validation of the thesis that hydroxyl topology controls the strength of the Stokes-Induced Stark Effect in hybrid flavonoid–semiconductor interfaces, establishing Ω_{OH} as a predictive structure-based control parameter for interfacial electrostatic and quantum behavior.

Figure 7(a–c) presents the quantitative relationship between the hydroxyl-topology descriptor Ω_{OH} and three coupled physical quantities: (a) excited-state dipole change $\Delta\mu$ (D), (b) Stokes-induced electric field E_{SISE} (GV m^{−1}), and (c) ESIPT timescale τ_{ESIPT} (fs), across the flavonoid series, with parameter values derived from Table 3.

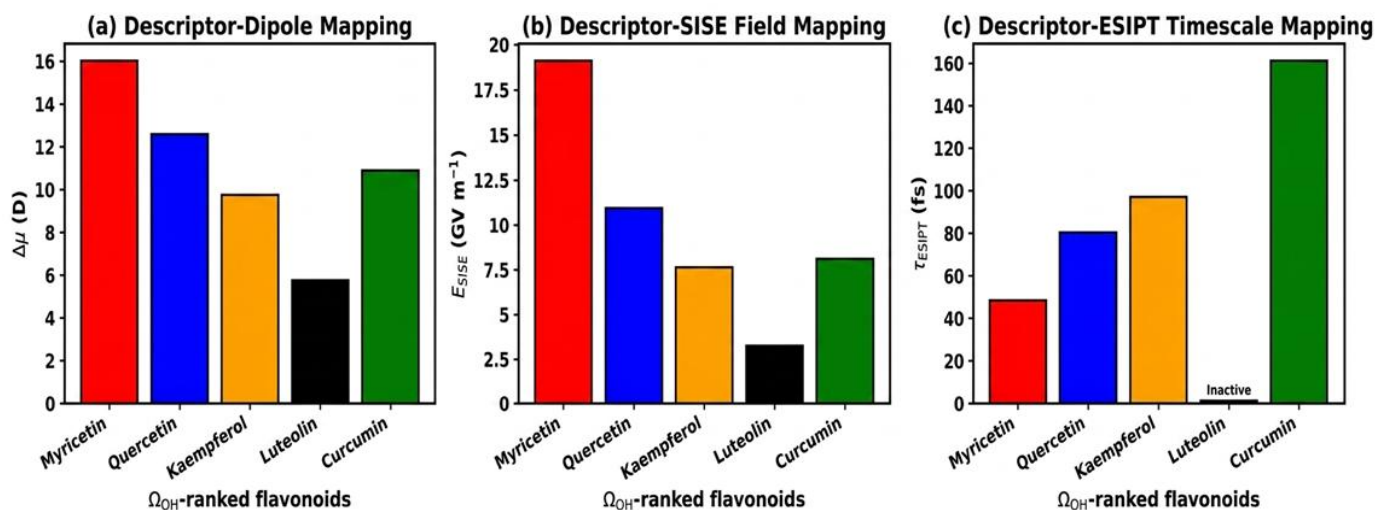


Figure 7(a–c): Descriptor-Mediated Mapping of Dipole, Field, and ESIPT Dynamics

A monotonic trend is observed in Figures 7(a) and 7(b), where both $\Delta\mu$ and E_{SISE} decrease systematically with decreasing Ω_{OH} . Myricetin exhibits the highest dipole moment change (~16 D) and strongest field (~19 GV m^{−1}), followed by Quercetin, Curcumin, and Kaempferol, while Luteolin shows the lowest values (~6 D and ~3 GV m^{−1}). In contrast, Figure 7(c) shows an inverse dependence, where higher Ω_{OH} corresponds to shorter ESIPT timescales (faster proton transfer), while lower descriptor values correspond to slower dynamics or complete suppression of ESIPT (Luteolin).

This trend arises from the direct coupling between hydroxyl topology and excited-state hydrogen-bond dynamics. Increased hydroxyl density enhances intramolecular hydrogen bonding networks, lowering proton-transfer barriers and enabling ultrafast ESIPT. This leads to significant charge redistribution and

dipole amplification, which in turn strengthens the interfacial electric field according to $E_{\text{SISE}} \propto \frac{\Delta\mu \cos \theta}{\epsilon_{\text{eff}} R^3} \sim \Omega_{\text{OH}}$. Thus, Ω_{OH} simultaneously encodes structural, dynamical, and electrostatic contributions to SISE generation.

These results are consistent with recent computational and spectroscopic studies showing that substituent effects and hydroxyl positioning strongly modulate ESIPT efficiency and excited-state dipole formation[44,58-59].

These results imply that hydroxyl topology does not merely correlate with dipole or ESIPT behavior but actively controls the entire chain of SISE generation, from ultrafast proton transfer to dipole amplification and ultimately to interfacial electric field strength. The simultaneous scaling of $\Delta\mu$, E_{SISE} , and τ_{ESIPT} with Ω_{OH} establishes a unified mechanistic framework, thereby providing direct quantitative support for the thesis that hydroxyl topology controls the strength of the Stokes-Induced Stark Effect in hybrid flavonoid–semiconductor interfaces.

Figure 8 presents the normalized interfacial response as a function of the hydroxyl-topology descriptor Ω_{OH} on a log–log scale, comparing the scaling behavior in the global Rosen–Morse regime and the local Airy regime. The horizontal axis shows Ω_{OH} over the range ~ 0.25 to 1.7 , while the vertical axis represents the normalized response quantity.

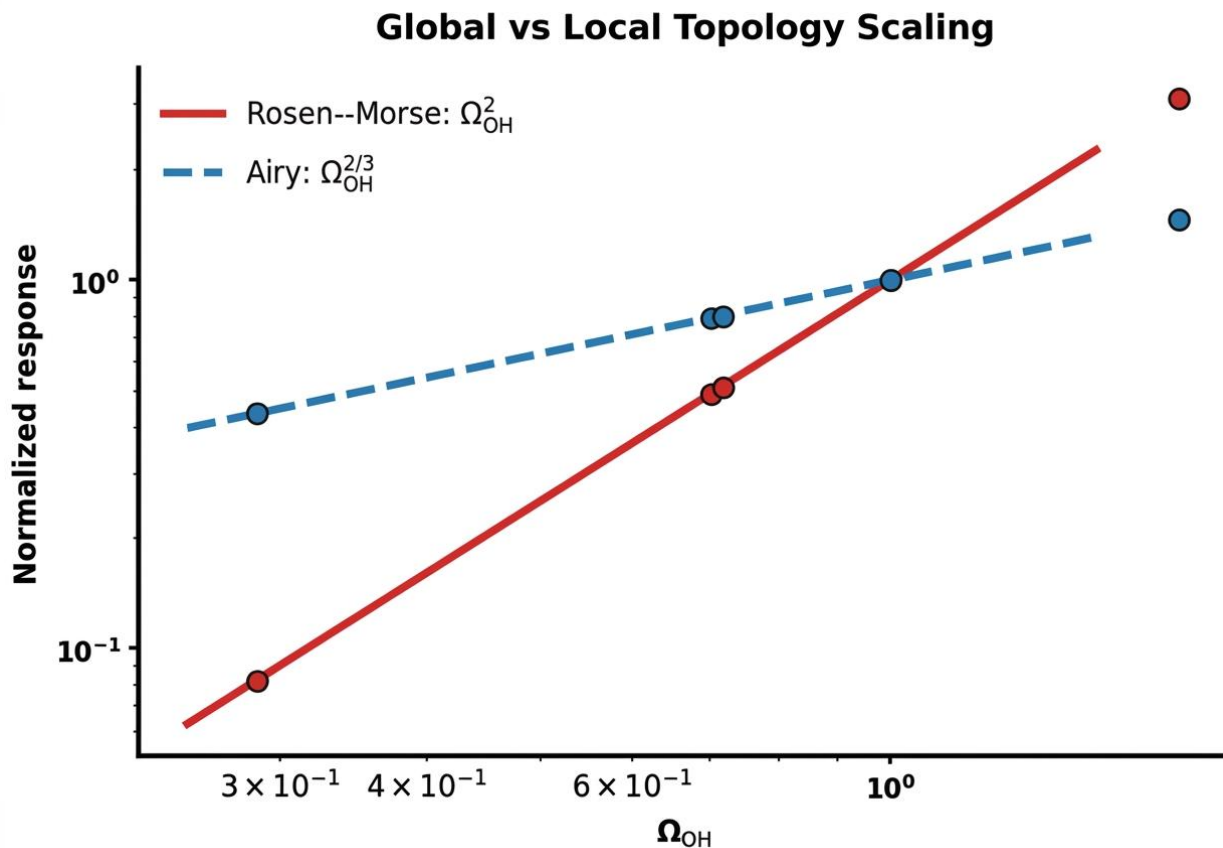


Figure 8: Global vs Local Topology Scaling of SISE Response

Two theoretical scaling laws are plotted viz a quadratic dependence $\propto \Omega_{\text{OH}}^2$ (solid red line) corresponding to the Rosen–Morse energy shift, and a sub-linear dependence $\propto \Omega_{\text{OH}}^{2/3}$ (dashed blue line) corresponding

to the Airy energy scaling. Discrete points represent the flavonoid systems mapped onto both scaling regimes.

A bifurcation in scaling behavior is observed. At lower values of Ω_{OH} , the response aligns more closely with the sub-linear Airy scaling, while at higher descriptor values, the response transitions toward the quadratic Rosen–Morse dependence. The slope difference in the log–log representation highlights the stronger sensitivity of the global regime to changes in hydroxyl topology compared to the local regime. Notably, the crossover region occurs near $\Omega_{OH} \sim 1$, where both scaling laws yield comparable magnitudes.

This behavior arises from the fundamentally different physics governing the two regimes. In the global regime, the energy shift is perturbative and follows $\Delta E_n^{RM} \propto E_{SISE}^2 \propto \Omega_{OH}^2$, leading to a quadratic amplification of the response with increasing descriptor. In contrast, the local regime is governed by strong-field triangular confinement, where the Airy quantization yields $E_n^{Airy} \propto E_{SISE}^{2/3} \propto \Omega_{OH}^{2/3}$, resulting in a weaker, sub-linear dependence. The log–log representation makes these scaling exponents explicit as linear slopes of 2 and 2/3, respectively.

This dual-scaling behavior is consistent with modern treatments of field-induced quantum confinement in nanoscale systems, where perturbative and strong-field regimes exhibit distinct power-law dependencies [56,57,60].

This result suggest that hydroxyl topology not only controls the magnitude of the Stokes-induced Stark field but also determines the scaling regime of the quantum response. Low-to-moderate descriptor values lead to weak-field behavior with Airy-type localization, while higher values drive the system into a regime where global energy shifts dominate with quadratic scaling. This establishes a unified structure–scaling relationship, confirming that Ω_{OH} acts as a governing parameter that dictates both the strength and the functional form of the SISE response, thereby providing strong quantitative validation of the thesis.

Figure 9(a–c) presents the sensitivity of the Stokes-induced electric field E_{SISE} (in GV m^{-1}) to variations in three governing parameters: (a) excited-state dipole moment $\Delta\mu$ (D) over the range $5 \leq \Delta\mu \leq 15\text{D}$, (b) orientation angle θ (degrees) over $10^\circ \leq \theta \leq 50^\circ$, and (c) interfacial separation distance R (Å) over $2.0 \leq R \leq 3.5\text{Å}$. Each panel isolates one parameter while holding the others constant, thereby explicitly illustrating its independent contribution to the SISE field.

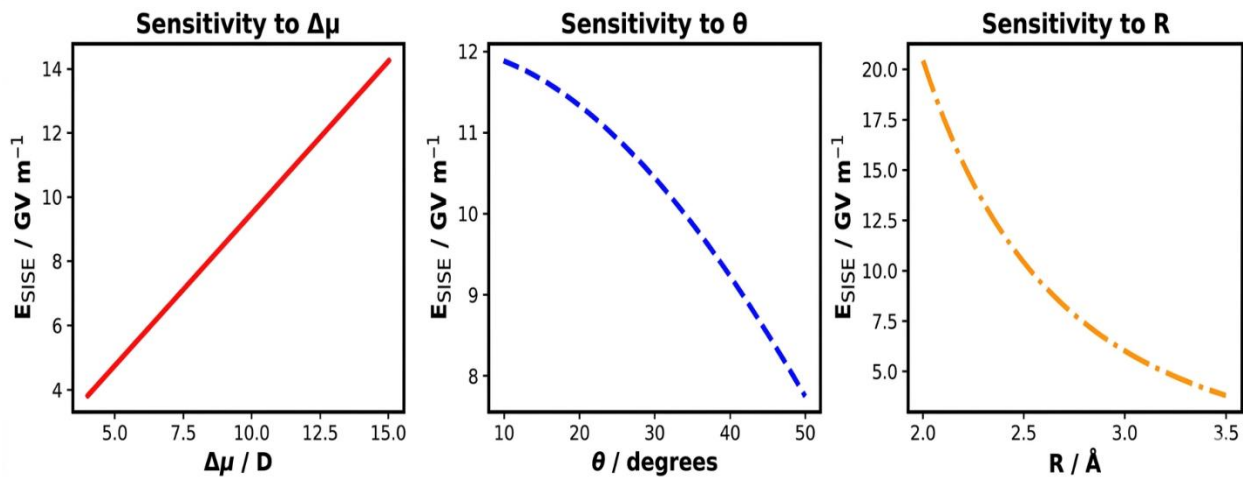


Figure 9(a–c): Sensitivity of SISE Field to Dipole, Orientation, and Distance Parameters

A quantitatively distinct trend is observed across the three panels. In Figure 9(a), E_{SISE} increases linearly with $\Delta\mu$, rising from approximately 4 to 14.5 GV m⁻¹, indicating a direct proportionality between dipole strength and field magnitude. In Figure 9(b), E_{SISE} decreases nonlinearly with increasing θ , dropping from about 11.8 GV m⁻¹ at 10° to ~ 7.7 GV m⁻¹ at 50°, reflecting the cosine dependence of the dipole projection along the interface normal. In Figure 9(c), the field exhibits the strongest sensitivity, decreasing sharply from ~ 20 GV m⁻¹ at $R = 2.0$ Å to ~ 4 GV m⁻¹ at $R = 3.5$ Å, demonstrating a steep inverse-cubic decay.

These trends arise directly from the electrostatic formulation of the SISE field, $E_{\text{SISE}} \propto \frac{\Delta\mu \cos \theta}{\epsilon_{\text{eff}} R^3}$. The linear dependence on $\Delta\mu$ explains the proportional increase in panel (a), while the angular dependence enters through the cosine projection, producing the nonlinear decrease observed in panel (b). The dominant contribution arises from the distance scaling R^{-3} , which amplifies small changes in interfacial separation into large variations in field strength, as seen in panel (c).

This result implies that the SISE field is most strongly controlled by interfacial distance, followed by dipole magnitude and orientation. Since the hydroxyl-topology descriptor Ω_{OH} incorporates all three parameters multiplicatively, it effectively captures the dominant physics governing field generation. This confirms that structural variations in hydroxyl arrangement influence SISE strength primarily through their impact on dipole formation, alignment, and spatial proximity, thereby providing mechanistic validation for the thesis that hydroxyl topology controls the strength of the Stokes-Induced Stark Effect in hybrid flavonoid–semiconductor interfaces.

Conclusion

In this work, we developed a quantum mechanical framework demonstrating how molecular architecture governs interfacial electrostatics and quantum behavior in hybrid flavonoid–semiconductor systems. By introducing the hydroxyl-topology descriptor Ω_{OH} , constructed from excited-state dipole dynamics $\Delta\mu$, orientational geometry θ , and interfacial separation R , we provide a deterministic mapping of the Stokes-Induced Stark Effect (SISE). Embedding this descriptor within a unified Rosen–Morse II and Airy-type formalism enable a consistent treatment of both global confinement and local field-dominated regimes, thereby capturing the energy shifts and wavefunction localization that characterize hybrid interfaces.

The results establish Ω_{OH} as a predictive control parameter for interfacial quantum response. Two distinct scaling regimes emerge: a quadratic dependence $\Delta E_n \propto \Omega_{\text{OH}}^2$ in the global perturbative limit, and a sub-linear scaling $E_n \propto \Omega_{\text{OH}}^{2/3}$ in the local Airy regime associated with strong-field triangular confinement. Wavefunction analysis supports this transition, showing that spatial profiles remain largely invariant in the global regime but exhibit pronounced localization and asymmetry in the local regime, with localization length scaling as $\ell \propto \Omega_{\text{OH}}^{-1/3}$. Sensitivity analysis further identifies interfacial distance as the dominant factor governing field strength, followed by dipole magnitude and orientation, all of which are encapsulated within the descriptor.

Despite these results, the present model is subject to several limitations. The formulation assumes a one-dimensional interfacial coordinate and quasi-static electric fields, neglecting multidimensional effects, dynamic disorder, and explicit non-adiabatic coupling during ES IPT. Environmental influences such as dielectric heterogeneity, phonon interactions, and surface defects are incorporated only implicitly. Addressing these limitations will require extension to multidimensional quantum treatments, incorporation of time-dependent fields, and integration with atomistic simulations such as DFT or QM/MM approaches. Experimental validation through ultrafast spectroscopic techniques, particularly

electroabsorption measurements, will be critical for confirming the predicted scaling relationships under realistic conditions.

This study provides a formalization of SISE as a predictive, structure-governed phenomenon. By establishing a unified structure–field–energy–wavefunction relationship, we show that hydroxyl topology serves as a fundamental determinant of interfacial quantum behavior. This provides a quantitative framework for rational molecular design, shifting hybrid optoelectronic systems from empirically tuned architectures toward descriptor-driven engineering. Thus, the results offer a foundational basis for the development of bio-inspired, field-tunable semiconductor interfaces with controllable quantum response.

Ethics approval and consent to participate

Not Applicable

Consent for publication

Not Applicable

Availability of data and material

Data sharing not applicable to this article as all datasets were generated and analyzed during the current study are based on the formulation within the study. Codes used for computation and visualization can be found here <https://github.com/Udoisohm/Hydroxyl-Topology-/releases/new>

Competing interests

The authors declare that they have no competing interests

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Authors' contributions

MU – Conceptualization, formulation, Computation, formal analysis, manuscript draft and revisions

KAB - manuscript review and analysis

MCN – Chemical Analysis, Review and revisions

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