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Mechanisms of perylene pre-nucleation on Ni(111) and SiO_2(0001) surfaces

D. Husanova *[1], **D. Boymamatova** [1], **S. Mehdi Vaez Allaei** [2], **S. Mirzaev** [1], **U. Khalilov** [3]

[1] Academy of Sciences of Uzbekistan, Arifov Institute of Ion-Plasma and Laser Technologies, Tashkent, 100125, Uzbekistan
[2] Department of Physics, University of Tehran, Tehran, 14179-35840, Iran
[3] MOSAIC Research Group, University of Antwerp, Antwerp, 2020, Belgium
dilfuzahusanova75@gmail.com (D.H.), boymamatovadildora99@gmail.com (D.B.), smvaez@gmail.com (S.M), szmirzaev@gmail.com (S.M.), ukhalilov@uantwerpen.be (U.Kh.)
* Correspondence: dilfuzahusanova75@gmail.com Tel.: +998 99 881 75 03 (D.H.)

Abstract: Organic semiconductor thin films are crucial for next-generation electronics, yet their early-stage nucleation on inorganic substrates is poorly understood. We employ reactive molecular dynamics simulations to study the pre-nucleation (clustering) of perylene on Ni(111) and SiO_2(0001). Strong chemisorption on Ni(111) stabilizes a flat-lying wetting layer (Stranski–Krastanov mode), whereas weak adhesion and strong π–π cohesion on SiO_2(0001) directly yield vertically oriented 3D islands (Volmer–Weber mode). Thermodynamic analysis of cohesive energy and molar Gibbs free energy quantitatively supports these transitions, providing a predictive framework for designing stable organic–inorganic interfaces.

Keyword: Perylene, reactive molecular dynamics, pre-nucleation, organic–inorganic interfaces, Stranski–Krastanov, Volmer–Weber.

Introduction

The integration of organic semiconductor materials into electronic devices opens significant opportunities for next-generation technologies, including organic light-emitting diodes (OLEDs) and organic field-effect transistors (OFETs) [1–5]. The efficiency and functional characteristics of such devices largely depend on the structure of the thin films formed by organic molecules on the substrate surface. In this context, the rational design of promising advanced materials relies heavily on the predictive power of atomistic modeling. Predicting the thermodynamic and kinetic behavior during molecular clustering (pre-nucleation, i.e., the initial stage of film growth) is crucial for tailoring the morphology and macroscopic properties of the resulting nanostructures [6–9].

In thin-film devices, the orientation of perylene molecules, intermolecular interactions, and interaction with the substrate significantly influence device performance, especially during the pre-nucleation (clustering) stage, which involves the formation of initial crystalline nuclei. Therefore, studying the mechanisms of nanostructure formation, including clustering kinetics and surface adsorption, is of fundamental importance for the development of organic electronics. Despite significant progress in studying perylene thin-film growth on metallic substrates [10–17], its adsorption on oxidized and semiconductor surfaces remains insufficiently explored, particularly regarding the initial clustering stage that determines subsequent crystal growth [18–20]. However, understanding the clustering mechanisms on these surfaces at the atomic level is not merely about explaining existing experimental phenomena; rather, it is about unlocking the predictive capability to design highly stable organic-inorganic interfaces for future devices [21,22]. By simulating these early stages, researchers can predict whether an adsorbat will form homogeneous layers or isolated clusters before any physical synthesis takes place. Nickel (Ni), characterized by high thermal conductivity and catalytic activity, represents a promising platform for studying perylene-surface interactions, especially during the initial stages of pre-nucleation [23,24]. The morphology of Ni(111) surfaces significantly impacts

Quoting: D. Husanova, D. Boymamatova, S. Mehdi Vaez Allaei, S. Mirzaev, U. Khalilov. Mechanisms of perylene pre-nucleation on Ni(111) and SiO_2(0001) surfaces. **2026**, 3, 1, 5. https://doi.org/

Received: 11.01.2026
Corrected: 30.01.2026
Accepted: 05.02.2026
Published: 28.02.2026

the adsorption and clustering of perylene molecules [7,25]. While silicon (Si) also offers a flexible interface for studying these processes [26], the thermodynamic and kinetic factors controlling perylene nucleation on these surfaces, particularly at the pre-nucleation stage, are not yet fully understood.

In this work, the clustering processes of perylene molecules on two fundamentally different surfaces, i.e., metallic Ni(111) with high catalytic activity and dielectric SiO_2(0001), are compared using the reactive molecular dynamics (MD) method. The goal of the study is to determine, at the atomic level, the influence of the substrate type on perylene adsorption, molecular orientation, growth modes and the thermodynamic stability of the resulting layers. Ultimately, this comparative analysis aims to establish a predictive computational framework for the targeted synthesis and integration of promising nanoscale materials in advanced electronic applications.

Materials and Methods

The clustering mechanisms of perylene ($C_{20}H_{12}$) molecules on monocrystalline Ni(111) and SiO_2(0001) surfaces were investigated using reactive molecular dynamics (MD) simulations with the LAMMPS software package [27]. To accurately capture the complex interfacial chemistry without the immense computational cost of ab initio methods, interatomic interactions were modeled using the ReaxFF reactive force field [28]. Specifically, the parameter sets developed by Zou et al. [29] for the Ni–C–O–H system and by Newsome et al. [30] for the Si–C–O–H system were utilized. These parametrizations, originally derived from quantum mechanical data, provide a chemically realistic description of bond formation, bond dissociation, and dynamic charge transfer. Furthermore, they capture non-bonded van der Waals and electrostatic interactions, which are critical for predicting the π–π stacking of perylene and its adhesion to the substrates [31].

The simulated systems comprised perylene molecules deposited on monocrystalline Ni(111) and α-quartz SiO_2(0001) slabs. α-Quartz, the stable polymorph of SiO_2, has a well-defined piezoelectric (0001) surface whose polarization and associated electric fields can influence molecular adsorption and interfacial behavior. The substrate structures were constructed using the VESTA program [32], and the surface dimensions of 24.97×25.20 Å^2 for Ni(111) and 24.95×25.93 Å^2 for SiO_2(0001). Periodic boundary conditions were applied in the x and y directions to mimic macroscopic surface conditions, while a sufficient vacuum gap was introduced in the z-direction to prevent spurious interactions between periodic replicas.

The initial geometries of the substrates were optimized by sequentially applying the steepest descent and conjugate gradient energy minimization algorithms. Subsequently, the systems were gradually heated to 300 K at a rate of 1 K/ps using an isothermal-isobaric (NpT) ensemble controlled by a Nosé–Hoover barostat and thermostat [33,34]. Thermodynamic equilibrium was then established and maintained at 300 K under a canonical (NVT) ensemble.

Following equilibration, perylene molecules were sequentially deposited onto the target surfaces every 0.25 ns. This deposition rate corresponds to an effective molecular flux of approximately 6.3 10^{26} s^{-1} m^{-2}. The system temperature was rigorously maintained at 300 K using the Nosé–Hoover thermostat, with the temperature continuously monitored every 100 fs. The reactive MD simulations were conducted for a total duration of 40 ns, comprising 160 million integration steps with a time step of 0.25 fs.

To quantitatively evaluate the thermodynamic stability of the evolving thin films and the interaction strength of the formed nanoclusters, the cohesive energy and molar Gibbs free energy of the systems were extracted. The cohesive energy per perylene molecule within the cluster, E_{coh} was calculated using the standard difference expression:

$$E_{coh} = \frac{E_{total}}{n} - E_{mol} \tag{1}$$

where E_{total} represents the time-averaged total potential energy of the fully equilibrated molecule–substrate system, n is the number of perylene molecules deposited on the surface, and E_{mol} corresponds to the potential energy of a single isolated perylene molecule optimized in a vacuum under the same ReaxFF conditions.

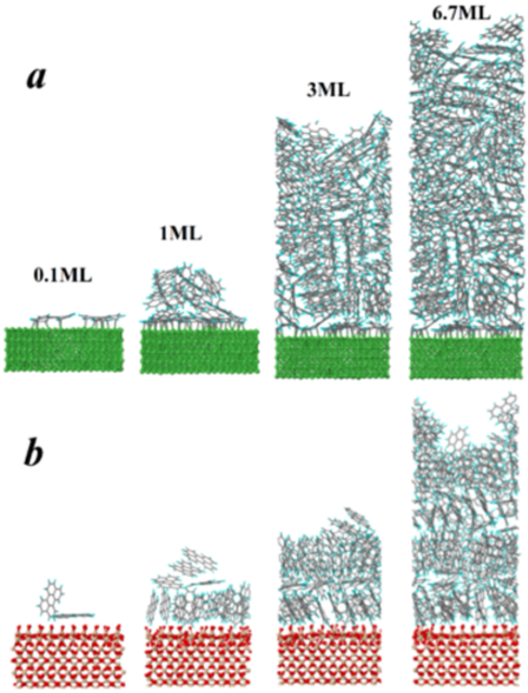

Figure 1. *Sequential deposition of perylene molecules on the (a) Ni(111) and (b) SiO_2(0001) surfaces.*

Furthermore, the relative thermodynamic stability of the perylene networks on the Ni and SiO_2 surfaces was evaluated via the molar Gibbs free energy (ΔG_m) change of formation, derived from their final potential energies [35]:

$$\Delta G_m = E_{coh} - \sum \chi_i \mu_i \tag{2}$$

where χ_i denotes the fractional concentration of the i-th atomic species (C, H, Ni, Si, and O) in the system, and and μ_i corresponds to the chemical potential of that species in its standard bulk reference state.

Results

Figure 1 illustrates the dynamic simulation results of the sequential deposition and clustering of perylene molecules on the Ni(111) and SiO_2(0001) surfaces at various coverages (0.1, 1, 3, and 6.7 ML). The visual analysis of the molecular trajectories reveals a profound substrate-dependent dichotomy in both the preferred orientation of the adsorbed molecules and the overall morphological evolution. On the highly catalytic Ni(111) surface (Fig. 2a), the strong chemisorption, i.e., driven by the extensive hybridization between the surface Ni d-orbitals and the conjugated π-electron system of perylene, forces the molecules to adopt a strictly flat-lying (surface-parallel) orientation during the initial stages of deposition (0.1 and 1 ML). This configuration maximizes the interfacial contact area, minimizing the surface energy and forming a well-ordered, continuous wetting layer. As the film thickness increases to 3 ML and ultimately reaches 6.7 ML, the direct electronic influence of the metallic substrate rapidly decays, allowing intrinsic intermolecular π–π stacking forces to become dominant.

Consequently, the molecules in the upper layers undergo a distinct structural transition, adopting tilted or nearly vertical orientations and agglomerating into three-dimensional (3D) islands over the initial flat layers. This progressive transition from layer-by-layer growth to island formation visually confirms the realization of the Stranski–Krastanov (SK) growth mode [36,37].

In stark contrast, on the dielectric SiO_2(0001) surface (Fig. 2b), the weak interfacial physical interactions are easily overcome by the strong intrinsic cohesive forces between the planar molecules. Consequently, the formation of an initial wetting layer is entirely bypassed. Even at the earliest sub-monolayer coverages (0.1 ML) and up to 1 ML, rather than spreading out, the perylene molecules immediately adopt a vertical or highly tilted orientation relative to the substrate surface, optimizing intermolecular π–π stacking from the very onset of the deposition. As the deposition continues through 3 ML to 6.7 ML, this vertical stacking preference rigidly persists, resulting in the rapid and sustained growth of isolated 3D clusters. This direct island formation without any preceding wetting layer is the hallmark of the Volmer–Weber (VW) growth mode [38].

Thus, Ni(111) promotes a two-stage SK-type growth (initial wetting layer followed by 3D islands), whereas SiO_2(0001) directly undergoes a VW-type 3D island growth without a wetting layer already at sub-monolayer coverage. The distinct morphological differences and molecular orientations observed in these simulations highlight the critical role of substrate selection in the predictive modeling and rational design of promising organic–inorganic interfaces.

To quantitatively substantiate these substrate-dependent growth modes and the preferred molecular orientations observed in Fig. 1, we next analyzed the thermodynamic driving forces governing the clustering processes. Figure 2 depicts the dependence of the molar Gibbs free energy (ΔG_m) and cohesive energy (E_{coh}) of perylene molecules on the film thickness (0–7 ML) deposited on Ni(111) and SiO_2(0001) substrates. The molar Gibbs free energy (Fig. 2, solid lines) exhibits a pronounced initial increase for both systems as the coverage expands. On the SiO_2(0001) surface, ΔG_m rises from approximately 6.20 eV at the initial stage to about 6.80 eV within the first monolayer (1 ML), while on Ni(111) it increases from roughly 6.10 eV to 6.70 eV over the same range. Beyond 1 ML, the growth rate of ΔG_m progressively decelerates and eventually plateaus near 7.10 eV at 7 ML for both substrates. This plateau signifies a thermodynamic transition towards the structural stabilization of a bulk-like perylene phase, where the energetic contribution of the underlying substrate becomes negligible.

Concurrently, the cohesive energy of the perylene clusters (Fig. 2, dashed lines) provides critical insight into the competition between intermolecular interactions and molecule–substrate adhesion. As the film thickness increases, E_{coh} rapidly shifts to more negative values, indicating enhanced intermolecular binding within the growing perylene network. On the SiO_2(0001) substrate, E_{coh} attains a highly negative value of approximately -1.15 eV at 1 ML, compared to about -1.05 eV on the Ni(111) surface. The stronger cohesion on SiO_2(0001) at 1 ML ($E_{coh} \approx -1.15$ eV) compared to Ni(111) ($E_{coh} \approx -1.05$ eV) indicates that intermolecular interactions dominate over molecule–substrate adhesion on the oxide, providing the energetic driving force for VW-type 3D island growth. This stronger cohesion among perylene molecules on SiO_2, which effectively outweighs the molecule–substrate adhesion, promotes rapid agglomeration into three-dimensional islands, characteristic of the VW growth mode.

Conversely, the comparatively weaker cohesion of perylene on Ni(111) at 1 ML ($E_{coh} \approx -1.05$ eV) reflects a much stronger competing molecule–substrate chemisorption. This energetic balance stabilizes flat-lying configurations and enforces the formation of an initial wetting layer, which is a defining feature of the SK growth mode. Notably, beyond approximately 3 ML, the cohesive energies for perylene on both substrates converge to around -1.40 eV and ultimately stabilize near -1.45 eV at 7 ML. Beyond approximately 3–4 ML, ΔG_m and E_{coh} for Ni(111) and SiO_2(0001) become nearly identical. This indicates that once a critical thickness is exceeded, the film behaves essentially as bulk perylene, and the substrate mainly controls only the initial nucleation pathway rather than the properties of the thick film. This convergence clearly demonstrates that at higher coverages the energetic influence of the substrate is fundamentally diminished, and the cohesive properties of the film become predominantly governed by the intrinsic π–π intermolecular forces of the bulk perylene network.

Overall, the energetic analysis establishes a direct link between the thermodynamic driving forces and the observed growth modes. On Ni(111), the comparatively weaker cohesion at 1 ML reflects strong molecule–substrate chemisorption, enforcing the formation of a wetting layer and thus an SK-type growth pathway. In contrast, the stronger cohesion on SiO_2(0001) already at sub-monolayer coverage favors the immediate aggregation into vertically stacked 3D islands, i.e., a VW-type growth regime. These energetic profiles quantitatively corroborate the morphological observations, demonstrating that the competition between molecule–substrate chemisorption and intermolecular cohesion uniquely selects the SK or VW growth mode on the respective substrates.

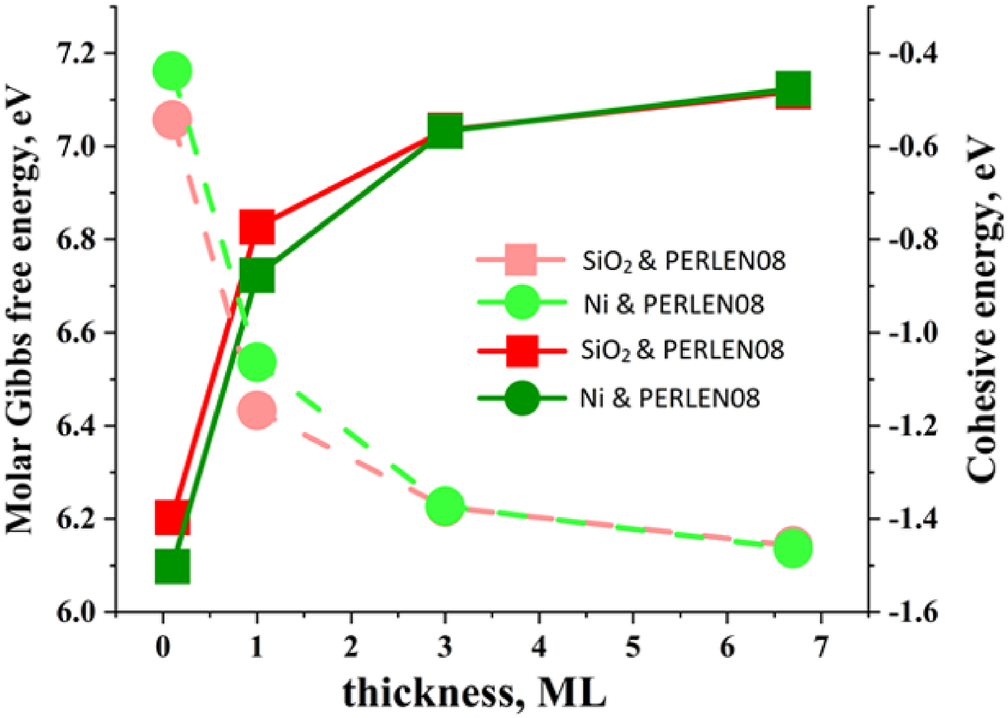

Figure 2. *Dependence of the molar Gibbs free energy (solid lines) and cohesive energy (dashed lines) of perylene clusters on the film thickness deposited on Ni(111) and SiO_2(0001) substrates.*

Conclusions

Reactive molecular dynamics simulations were successfully employed to elucidate the early-stage pre-nucleation and clustering mechanisms of perylene molecules on Ni(111) and SiO_2(0001) surfaces. These results demonstrate the strong predictive capability of atomistic modeling for describing the morphological evolution and preferred molecular orientation in organic thin films. On the highly catalytic Ni(111) surface, strong molecule–substrate chemisorption dominates the initial stages, forcing perylene molecules into a flat-lying configuration and stabilizing a continuous wetting layer, which is a defining feature of the Stranski–Krastanov growth mode.

Conversely, on the dielectric SiO_2(0001) surface, relatively weak interfacial adhesion allows strong intrinsic intermolecular π–π cohesive forces to prevail from the outset. This balance drives the rapid formation of vertically oriented, isolated 3D clusters without any preceding wetting layer, directly giving rise to a Volmer–Weber island growth mode. Comprehensive thermodynamic analyses of the cohesive energies and molar Gibbs free energies quantitatively corroborate these distinct structural transitions. Overall, the insights obtained from this comparative study establish a practical computational framework for predicting interface stability and support the rational design and targeted synthesis of promising organic–inorganic hybrid materials for next-generation electronic applications.

Authors’ contribution

Conceptualization, U.K.; methodology, D.H., D.B., S.M.V.A. and S.M.; software, D.B., S.M.V.A. and S.M.; validation, D.B., S.M.V.A. and S.M.; formal analysis, D.H., D.B., S.M.V.A. and S.M.; investigation, D.H., D.B., S.M.V.A. and S.M.; resources, U.K.; data curation, D.B., S.M.V.A. and S.M.; writing—original draft preparation, D.H.; writing—review and editing, U.K.; visualization, D.H., D.B., S.M.V.A. and S.M.; supervision, U.K.; project administration, U.K. All authors have read and agreed to the published version of the manuscript.

Funding source

The results presented in this article were obtained with the financial support of the Fundamental Research Project No. F-FA-2021-512.

Ethics approval.

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Consent for publication

This article does not contain any studies with human participants or animals performed by any of the authors.

Data Availability Statement

Statement of informed consent was not required as no human subjects were involved in this research.

Acknowledgments

All experimental data confirming the results presented in this article are held by the authorsand presented within the article in the form of the main text and image. Additional informationcan be obtained from the author(s)based on a reasoned query.

Conflict of interest

This research was carried out within the framework of scientific programs supported by the Academy of Sciences of Uzbekistan and financed from the state budget of Uzbekistan. Also, the authors acknowledge financial support from the Agency for Innovative Development of the Republic of Uzbekistan

Abbreviations

MD	Molecular dynamics
ReaxFF	Reactive force field
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
Ni	Nickel
SiO_2	Silicon dioxide
OLEDs	Organic light-emitting diodes
OFETs	Organic field-effect transistors
SK	Stranski–Krastanov growth mode
VW	Volmer–Weber growth mode
ML	Monolayer
NVT	Canonical ensemble
NpT	Isothermal-isobaric ensemble
E_{coh}	Cohesive energy
ΔG_m	Molar Gibbs free energy

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