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From Fibrated Chrysene Networks to Molecular Machines

Registry-Programmed Geometry, Electromechanical Realization, and Constructive Existence

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Abstract

The fibrated architecture of the Chrysene Formalism provides a labelled reference network with substituent-mediated lateral connections and a distinct interlayer stacking relation. We extend a finite portion of that architecture into a registry-dependent mechanical system by assigning molecular positions, orientations, compliant connector coordinates, interaction energies, and admissible transitions. The integer address, physical configuration, local structural tensor, and numerical mesh are kept distinct. General results establish constrained equilibrium existence, local stable branches, controlled dissipation, symmetry obstructions, and compatibility of finite executions.

A constructive reduced realization consists of two eight-core stacked patches joined through a compliant aperture. One common energy yields its equilibrium aperture and its state-dependent binding levels. A declared electrostatic registry coupling produces target discrimination; a controlled aperture change produces capture and release. An explicit parameter choice has target occupancy greater than 0.98 in the capture setting and empty-site probability greater than 0.97 in the release setting. These strict inequalities, the geometric clearance, and the positive reduced stiffness persist in a neighborhood of the model parameters. Reversible binding kinetics and a mechanical relaxation law complete the finite operational model without identifying equilibrium motion with directed work.

We then define compatible interfaces for coupled code–product formation and structure-filtered peptide selection, prove a finite coding-lift result and a selection leakage bound, and organize hinges, gates, sliders, pockets, rotors, and helicase-like assemblies into an atlas of proof obligations. A posteriori mechanical bounds distinguish numerical verification from continuum homogenization. The existence result concerns an explicitly specified coarse molecular model; molecular calibration, reaction chemistry, and autonomous assembly constitute further realization problems.

Keywords: Chrysene Formalism; fibrated network; molecular machine; programmable metamaterial; registry; constrained mechanics; capture and release; constructive existence; peptide selection.

1 Introduction

An encoded molecular architecture becomes a machine only when its structural organization supports a reproducible action. For substituted chrysene assemblies, the proposed construction has two complementary ingredients: connections through the $3, 6, 9, 12$ attachment sites organize lateral structure, while interactions between stacked aromatic cores provide an interlayer coupling. Together they suggest a three-dimensional material whose local organization can be indexed and programmed. The purpose of this paper is to give that proposal an explicit mechanical interpretation and a constructive existence theorem for its first elementary function: selective capture followed by controlled release.

The revised twelve-axiom formalism separates the molecular node, directional bridges, tensor-network architecture, sequence algebra, spectral geometry, and physical response [Sch26b]. Its discrete fibration supplies an indexing structure, not a constitutive mechanical law. The metamaterial study motivates substituent-linked patches, stacked columns, and reactive interstitial environments [Sch26h]. Their combination suggests a node-based mechanical description comparable in organization to a discrete structural solver: a node carries position and orientation, a connection carries an interaction law, and an interstitial region acquires its geometry from the configurations of its boundaries. The molecular graph nevertheless remains distinct from any auxiliary numerical mesh.

Four preceding pilot constructions establish the context. The genetic-code study organizes a typed chrysene–adenosine carrier, variable coding data, and a formal product grammar [Sch26c]. The protocell study develops material-accounted interfaces between assembly, preparation, production, and operation

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[Sch26a]. The finite interior-chrysene-lattice study introduces native component geometries, formal catalytic realizations, and a common functional model [Sch26e]. The source comparison places endogenous assembly and exogenous preparation within shared configuration and operational spaces [Sch26d]. The present article initiates a molecular-machine series by linking reference geometry, mechanical deformation, and binding function within a single specified realization.

The distinction between structure and function is productive rather than merely restrictive. Once an interaction model is fixed, one can ask which modes are stabilized, which coordinate remains controllable, which substrate is preferentially retained, and which operation restores an available binding site. A fully rigid mesh provides a structural body; a deliberately compliant subregion provides a candidate mechanism. The challenge is to stabilize the body without eliminating the mechanism or allowing uncontrolled collapse.

Experimental molecular-machine research demonstrates the importance of the corresponding distinction between motion and energy transduction. DNA-origami rotary ratchets use an external drive to bias motion [PEK+22]; a catalysis-driven artificial motor has performed work against a load through chemical energy transduction [WBP+25]. These examples motivate explicit control and energy accounts. They are not experimental realizations of the chrysene construction studied here.

1.1 Contribution and logical scope

Our main contribution is a finite *mechanical realization lift*: a labelled fibrated reference architecture is supplied with positions, orientations, interaction laws, and operational states on one common configuration space. We prove general local results and construct an explicit sixteen-core reduced gate. Its energy determines both its equilibrium aperture and the binding levels used by its finite occupancy model. Thus the mechanical and functional coefficients are not unrelated choices introduced in separate examples.

The electrostatic projection, elastic constants, exclusion geometry, and kinetic rates are constitutive data of this model. Their numerical values are dimensionless witnesses, not fitted chrysene measurements. The theorem establishes a nonempty robust class of the declared models. A molecular realization additionally requires calibrated interactions and chemically admissible connectors and state transitions. This boundary is recorded once in the hypotheses and retained throughout the proofs.

The peptide routes and the machine atlas are included as explicit interfaces. The article proves a selection bound, a finite encoding lift, and a conditional composition result; it does not identify every atlas entry with an already constructed molecule. In particular, code–product co-formation, proton-coupled electron transfer (PCET), and sustained strand unwinding retain their own mechanistic certificates.

1.2 Source precedence

The revised axioms govern inherited mathematical claims. The primary directions are linearly independent and inequivalent, but need not be perpendicular. A reference stacking edge is not itself a proof of a particular stacking potential, and a four-state alphabet does not imply four physical cavity shapes. The older metamaterial architecture is therefore used as design motivation, not as a substitute for the explicit energetic hypotheses below. Likewise, the infinite spectral construction is not transferred unchanged to a finite mechanical network, and its Dirac operator is not a stiffness matrix. This convention preserves the layered structure of the revised formalism while allowing new constitutive realizations.

2 Finite inheritance and mechanical state

2.1 Reference architecture and the two fibrations

The revised axiomatic foundation [Sch26b] distinguishes the embedded molecular node, its labelled attachment directions, bridge closure, the stacking relation, and subsequent operator realizations. We retain that separation. In particular, the directions $3 \to 9$ and $12 \to 6$ are linearly independent but need not be orthogonal. The architectural proposals in [Sch26h, Sections 3–4] motivate distinct lateral and stacking interactions; their constitutive laws are specified below rather than inferred from the index lattice.

Definition 2.1 (Finite decorated reference)**.** Let $\Lambda \subset \mathbb{Z}^3$ be finite and nonempty. Fix a labelled rigid molecular core with reference atomic positions $r_v \in \mathbb{R}^3$, including four ports r_3, r_9, r_{12}, r_6. Choose

$$L = (a_x\ a_y\ a_z), \qquad \det L \neq 0,$$

and put $x_k^0 = Lk$ for $k \in \Lambda$. For $\alpha \in \{x, y, z\}$ let

$$E_\alpha \subset \{(k, k + e_\alpha) : k, k + e_\alpha \in \Lambda\}.$$

An x-edge joins port 9 to port 3, and a y-edge joins port 6 to port 12, with specified bridge and terminal data satisfying reference closure. An edge in E_z carries a stacking label $\eta_e \in \mathbb{Z}_2$ and a reference stacking relation, not an additional covalent bond by convention. Specified boundary attachments and any additional machine connectors form part of the data. The reference atomic embedding is

$$(k, v) \longmapsto x_k^0 + r_v.$$

It is required to be injective. Each additional connector is separately typed and is not silently added to the inherited nearest-address edge sets.

Proposition 2.2 (Finite restriction)**.** *Restriction of an injectively embedded axiomatic reference network to* Λ *preserves its molecular labels, the ordered ports, the stacking labels on retained edges, and every closure identity belonging to a retained lateral bridge. The restricted atomic sites have a positive minimum pairwise separation whenever there are at least two such sites.*

Proof. Restriction of an injective map is injective. Every retained bridge has the same endpoints and reference displacement data as in the original network, so its closure identity is unchanged. Labels are restricted functions. The finite collection of distances between distinct retained atomic sites consists of positive numbers and therefore has a positive minimum. □

This proposition concerns atomic reference sites. Positive clearance between extended cores, connector curves, or a moving substrate is an additional condition. Deleting boundary edges does not furnish a termination chemistry; boundary terminations must be supplied when they are needed by the selected realization.

The projection $(i, j, k) \mapsto (i, j)$ gives finite subsets of the stacking fibers of the parent discrete fibration. Separately, the local tensor spaces of Axiom A6 give the restriction $\coprod_{k\in\Lambda}\{k\} \times T_k$. Neither construction is the mechanical state space introduced below. A finite restriction also does not inherit the infinite crossed-product representation or compact-resolvent statement unchanged. The parent A7–A9 framework can index finite observables without identifying its Dirac operator with a mechanical stiffness matrix.

Definition 2.3 (Programming data)**.** A programming field ρ assigns declared substituent, bridge, reference-registry, or control-interface data to specified nodes and edges. It includes η when appropriate but is not identified with η. The latter is the binary stacking label inherited from the axiomatic architecture. A node address is an identifier; the ability to set a local component of ρ physically is a separate actuation hypothesis.

2.2 A mechanical lift of the labelled network

Let $B \subset \mathbb{R}^3$ be a compact rigid-core envelope containing the reference atomic positions. At node k assign a center $x_k \in \mathbb{R}^3$ and an orientation $R_k \in \mathrm{SO}(3)$. Tether coordinates are collected in a finite-dimensional variable ξ. A discrete mode s records the selected bond topology, charge/protonation state, and occupancy information. In a fixed mode,

$$p_{k,v} = x_k + R_k r_v, \qquad B_k = x_k + R_k B. \tag{1}$$

Each bridge is represented by its specified endpoint-compatible configuration or curve, depending on the resolution of the model. Its endpoints are the physical ports in (1).

Definition 2.4 (Admissible mechanical state)**.** For fixed s and ρ, an admissible configuration is a tuple

$$q = ((x_k, R_k)_{k\in\Lambda}, \xi)$$

satisfying the declared boundary conditions, bridge constraints, noninterpenetration conditions, and mode-specific chemical guards. Write $\mathcal{Q}_{s,\rho}$ for its set. A physical state additionally includes the current control $u \in \mathcal{U} \subset \mathbb{R}^m$, and any substrate or reservoir coordinates used by the selected model. Different modes may have different configuration spaces and dimensions.

The reference configuration satisfies its chosen closure equations. A deformation need not satisfy $x_k = Lk$ at later times. The address, incidence, and protected molecular data persist while the embedding moves. Rotational degrees of freedom cannot generally be discarded: two equal center positions with different R_k give different port alignments.

Proposition 2.5 (Port covariance)**.** *Let* $g(y) = Qy + b$ *with* $Q \in \mathrm{SO}(3)$*. Under*

$$x_k \mapsto Qx_k + b, \qquad R_k \mapsto QR_k,$$

each port and core envelope is transformed by g*. Euclidean distances and endpoint-compatible bridge incidence are preserved when bridge configurations and boundary data are transformed by the same* g*.*

Proof. The transformed port is $Qx_k + b + QR_k r_v = g(p_{k,v})$. The same identity applied to every point of B proves the envelope assertion. Proper Euclidean motions preserve distances, and applying one map to a bridge and both endpoints preserves their equality. □

External fields must also be transformed when claiming covariance of field-dependent energies. A fixed laboratory field can intentionally break this symmetry.

The spaces $\mathcal{Q}_{s,\rho}$ are not asserted to be one global smooth manifold. Fixed-topology, fixed-contact regular regions admit smooth charts when their equality constraints have constant rank. Rank changes, active contacts, and topology changes must be treated separately. After fixing boundary conditions or a rigid-body gauge, let $y \in \Omega \subset \mathbb{R}^d$ be local independent coordinates on one such regular region, with configuration map $q = \chi(y)$. The local chart is the setting of the differential results below.

3 Constitutive realization and controlled mechanics

3.1 Interactions on the same configuration

The structural inheritance supplies incidence and reference data, not a force law. A constitutive realization assigns an energy to the same mechanical configuration and mode. A useful decomposition is

$$\begin{aligned} E(q; s, \rho, u) = {} & E_{\mathrm{bridge}}(q; s, \rho, u) + E_{\mathrm{stack}}(q; s, \rho) \\ & + E_{\mathrm{steric}}(q; s) + E_{\mathrm{elec}}(q; s, \rho, u) \\ & + E_{\mathrm{sub}}(q; s, \rho, u) + E_{\mathrm{bdry}}(q; u). \end{aligned} \tag{2}$$

Bridge energy can contain stretching, bending, and torsion. A stacking edge has local coordinates (h_e, t_e, ϑ_e) for separation, lateral slip, and relative orientation, and a separately declared potential

$$E_{\mathrm{stack}} = \sum_{e \in E_z} W_e(h_e, t_e, \vartheta_e; \eta_e).$$

The dimensions and charts of t_e and ϑ_e are part of the realization. Normal attraction alone does not control slip or twist. For example, near a chosen registered state a positive quadratic form in all these coordinates supplies a local stacking minimum; this is a constitutive assumption, not a consequence of the abstract z-edge.

Hard steric conditions may be included in $Q_{s,\rho}$ instead of a finite energy term. Charges, dielectric screening, protonation, and field coupling must be specified wherever they enter E_{elec}. The physical electronic Hamiltonians and dipole response of A10–A11 can supply a chosen subsystem only after its dependence on the present configuration is defined. The tensor or spectral description by itself determines neither this energy nor a barrier height.

For fixed (s, ρ) write $E_u(q) = E(q; s, \rho, u)$ and $e(y, u) = E_u(\chi(y))$. A Hessian of e is a local mechanical stiffness operator. A physically scaled mobility or mass matrix is additional data; it does not follow from a graph Laplacian merely because both are matrices indexed by nodes.

3.2 Existence of constrained equilibria

Theorem 3.1 (Compact-sublevel equilibrium)**.** *Fix u. Suppose $Q_{s,\rho}$ is a metric space, E_u is real-valued and lower semicontinuous, and some $q_0 \in Q_{s,\rho}$ has a compact nonempty sublevel set*

$$K = \{q \in Q_{s,\rho} : E_u(q) \le E_u(q_0)\}.$$

Then E_u attains its global minimum on $Q_{s,\rho}$.

Proof. Lower semicontinuity on nonempty compact K gives a minimizer $q_* \in K$. Its energy is at most $E_u(q_0)$. Every point outside K has strictly larger energy than $E_u(q_0)$, so q_* is also a global minimizer on the entire configuration space. □

A closed, bounded admissible configuration set in a finite coordinate model is one sufficient setting. More generally, coercivity together with closed admissibility and lower semicontinuity can establish compact sublevels. An exclusion condition of the form $d > 0$ is open, however; compactness cannot be inferred from boundedness alone if a minimizing sequence approaches forbidden contact.

The theorem is conditional and does not select a machine function. It neither proves nonemptiness of an unspecified molecular specification nor identifies the minimum with a desired pore or gate. A concrete realization must separately verify its geometric constraints and functional inequalities. The explicit construction below provides such a reduced-model witness.

3.3 Stable branches and functional margins

Theorem 3.2 (Regular controlled branch)**.** *Let $\Omega \subset \mathbb{R}^d$ and $\mathcal{U} \subset \mathbb{R}^m$ be open, and let $e \in C^2(\Omega \times \mathcal{U})$. Suppose*

$$\nabla_y e(y_0, u_0) = 0, \qquad H_0 = \nabla_y^2 e(y_0, u_0) > 0.$$

There are neighborhoods V of u_0 and O of y_0, and a unique C^1 map $y_* : V \to O$, such that $y_*(u_0) = y_0$ and $\nabla_y e(y_*(u), u) = 0$. After shrinking the neighborhoods, every $y_*(u)$ is a strict local minimum and its Hessian has a uniform positive lower eigenvalue bound.

Proof. Apply the implicit function theorem to $F(y, u) = \nabla_y e(y, u)$. Its derivative in y at the reference point is the invertible matrix H_0. This gives the asserted local branch and local uniqueness of stationary points. If $\lambda_0 > 0$ is the least eigenvalue of H_0, continuity of the Hessian permits neighborhoods on which its operator-norm difference from H_0 is less than $\lambda_0/2$. The quadratic form is therefore bounded below by $(\lambda_0/2)\|v\|^2$. The second-derivative criterion proves strict local minimality. □

The coordinates are independent constrained coordinates. Positive definiteness is required only after removing rigid-body gauge directions and imposing the declared constraints. Deliberate compliance is compatible with the theorem: a small but positive stiffness remains stable. An exactly neutral mechanism requires a separate treatment or must be designated as a control coordinate, not included in a supposedly positive-definite Hessian.

Proposition 3.3 (Persistence of strict performance margins)**.** *In the preceding setting let $g_1, \dots, g_N$ be continuous functions of (y, u) representing collision clearances, admissibility margins, or performance differences. If $g_j(y_0, u_0) > 0$*

for every j, then, on a possibly smaller neighborhood V, all $g_j(y_*(u), u)$ have positive lower bounds. The same conclusion holds with finitely many constitutive parameters adjoined to u, provided the hypotheses remain valid.

Proof. Each composition $u \mapsto g_j(y_*(u), u)$ is continuous and positive at u_0. Restrict to a neighborhood where it exceeds half its value at u_0, and intersect these finitely many neighborhoods. □

This is a local robustness result. For a prescribed finite control interval, coverage of the entire branch, nonvanishing stiffness, and positive margins must be established over that interval. No global opening path follows merely from a stable equilibrium at each of two endpoints.

Proposition 3.4 (Compact-path clearance)**.** *Let $\gamma : [0, 1] \to \mathcal{Q}_{s,\rho}$ be continuous and let $d_1, \dots, d_N$ be continuous admissibility margins. If $d_j(\gamma(t)) > 0$ for every t and j, their common minimum along the path is positive. If the path and margins depend jointly continuously on a finite parameter near a reference value, this positive clearance persists for all sufficiently small parameter perturbations.*

Proof. Take the minimum of finitely many positive continuous functions on the compact interval. Joint continuity on a compact interval gives a uniform neighborhood of the reference parameter on which the margins change by less than half this minimum. □

The proposition presupposes a supplied path. Two nonempty basins can lie in different connected components: for example $(-\infty, -1] \cup [1, \infty)$ admits no continuous path from -1 to 1. The operational construction must therefore supply reachability in addition to equilibrium existence.

3.4 Dissipative dynamics and work input

Definition 3.5 (Local overdamped realization)**.** On a fixed admissible chart let $M(y, u)$ be a C^1 symmetric positive-definite mobility matrix and let $u(t)$ be a C^1 control. The overdamped dynamics is

$$\dot{y} = -M(y, u(t))\nabla_y e(y, u(t)). \tag{3}$$

The mobility includes the coordinate metric and dissipation convention. Thus (3) is stated in the declared independent chart, not in redundant coordinates with constraints ignored.

Proposition 3.6 (Local flow and energy accounting)**.** *For every interior initial state, (3) has a unique local solution. Along that solution,*

$$\frac{d}{dt} e(y(t), u(t)) = -\nabla e^{\mathsf{T}} M \nabla e + \partial_u e \cdot \dot{u}, \tag{4}$$

where $\nabla e = \nabla_y e$. A solution extends over a finite control interval if it remains in a compact subset of the chart and the control remains in a compact subset of $\mathcal{U}$ over that interval.

Proof. The vector field is continuous in time and locally Lipschitz in y, giving local existence and uniqueness. The chain rule followed by substitution gives (4). Compact containment bounds the vector field and its local Lipschitz constants on a neighborhood of the trajectory; the standard continuation argument then extends the solution to the stated finite endpoint. □

The term $\partial_u e \cdot \dot{u}$ is supplied control power, and the first term is nonpositive dissipation. A closed cycle of material configuration is not a zero-cost cycle of the full apparatus. Chemical or electrical actuation requires its reservoir account. Discrete changes of s require guards, state maps, and separate energy/material balances; the continuous identity does not justify unaccounted jumps. Likewise, a moving energetic minimum is a quasistatic branch, not automatically the exact finite-speed solution of (3).

The finite-ICL framework [Sch26e] already distinguishes structural components and supplied operational laws. Here the additional requirement is that geometry, energy, stiffness, motion, and functional inequalities refer to one shared mechanical realization. That requirement is what makes the following explicit gate construction more than a juxtaposition of a lattice drawing and an independent state diagram.

4 An explicit layered capture–release gate

The general realization problem is now specialized to a finite witness. All lengths and energies in this section are nondimensional. The construction is an exact reduced mechanical model, not a numerical estimate of an actual chrysene binding energy. Its significance is that geometry, mechanical relaxation, registry-dependent contact, and functional selection are specified in one state space rather than in independent examples.

4.1 Sixteen indexed cores and a moving aperture

Let e_1, e_2, e_3 be the standard coordinate vectors, and set

$$a_x = (4, 0, 0), \qquad a_y = (1, 4, 0), \qquad a_z = (0, 0, 4). \tag{5}$$

These generators have determinant 64, and $a_x \cdot a_y = 4$. Thus the reference architecture is genuinely three-dimensional and its

in-plane coordinates are oblique. Use the finite address set

$$\Lambda_g = \{0,1,3,4\} \times \{0,1\} \times \{0,1\}. \tag{6}$$

The addresses with first coordinate 0, 1 form the left block; those with first coordinate 3, 4 form the right block. Within each block retain the nearest-address x- and y-connector edges and the z-stacking edges. Each block therefore contains eight molecular nodes, eight in-plane edges, and four stacking edges.

Fix one oriented reference core whose molecular positions lie in the closed unit ball about its center. The same orientation and the same ordered port labels are used at all nodes. For $i, j, k \in \{0,1\}$ define

$$q_{ijk} = (4i + j, 4j, 4k), \tag{7}$$

$$x^L_{ijk}(a) = q_{ijk}, \tag{8}$$

$$x^R_{ijk}(a) = q_{ijk} + (a+7)e_1, \qquad 2 \le a \le 6. \tag{9}$$

At $a = 5$, these are exactly the reference positions associated with (6) and (5). Away from that value the right block translates, but its molecular addresses and typed incidence remain unchanged. The moving configuration need not be a periodic lattice.

Proposition 4.1 (Core clearance and substrate corridor)**.** *For every $a \in [2,6]$, distinct core envelopes in (9) are disjoint and their mutual surface distances are at least 2. The left envelopes lie in $x \le 6$ and the right envelopes in $x \ge a+6$. A spherical substrate of radius $1/4$, whose center follows*

$$z_a(t) = (6 + a/2, t, 2), \qquad t \in \mathbb{R},$$

therefore has clearance at least $3/4$ from every core envelope.

Proof. Within one block, a nonzero center displacement is $(4\Delta i + \Delta j, 4\Delta j, 4\Delta k)$, where each difference is $-1, 0$, or 1. If $\Delta k \neq 0$ or $\Delta j \neq 0$, its norm is at least 4; otherwise its norm is 4. The unit envelopes consequently have surface separation at least 2. Their extremal left-block x coordinates are -1 and 6. Translating by $a + 7$ puts the right-block minimum at $a + 6$. A cross-block center separation is at least $a + 2 \ge 4$ in its x component. Finally the corridor center is at distance at least $a/2 \ge 1$ from either envelope half-space; subtracting the substrate radius gives the asserted clearance. □

The proposition concerns core envelopes and the stated substrate corridor. To define connectors, distinguish a molecular port from its exit from a conservative exclusion envelope. At the reference aperture $a = 5$, supply for every incident connector a port-to-exit attachment sleeve inside the collar of radius $5/4$ about its core center, ending at a distinct exposed anchor outside the unit ball. Intentional overlap of this sleeve with its incident envelope is permitted. The collars of different cores are disjoint, and at $a = 5$ they lie at distance at least $9/4$ from the reference corridor centerline. These are additional coarse geometric interface data, not an atom-resolved chemical chain or a newly inferred bond.

Exterior connector routes begin at the exposed anchors. They are chosen in the common exterior of the finitely many disjoint enclosing balls, outside a radius-one cylinder about the substrate centerline, with disjoint nonincident portions. Local exits in the collars and exterior piecewise-linear routes can be selected successively in three dimensions and put in general position; shared contact is allowed only in the declared incident attachment regions or junctions. This argument uses the ball-and-collar geometry of this witness, not a claim that arbitrary disjoint compact sets have accessible complements. Positive tube-clearance statements below apply to exterior portions and nonincident bodies; they do not demand exclusion from a connector's own attachment sleeve.

A continuous routing family can be fixed rather than reselected at each aperture. At $a = 5$ fix the attachment sleeves, exposed anchors, and exterior reference arcs just specified. Choose exterior arcs at distance at least 1 from the corridor centerline and with positive nonincident separation margins. Transport the sleeves, anchors, and arcs by $H_a(x, y, z) = (h_a(x), y, z)$, where

$$h_a(x) = \begin{cases} x, & x \le 6, \\ 6 + (a/5)(x-6), & 6 \le x \le 11, \\ x + a - 5, & x \ge 11. \end{cases}$$

This map fixes the left block, translates the right block exactly, and takes the reference centerline to $x = 6 + a/2$. It is a continuous family of bi-Lipschitz homeomorphisms with lower distance factor at least $2/5$. The transported arcs consequently retain a positive uniform separation and distance at least $2/5$ from the moving centerline. Choose tube radii smaller than half the minimum nonincident arc separation, smaller than the nonincident body clearance, and smaller than $3/40$. The substrate of radius $1/4$ then retains positive connector clearance as well. These piecewise-smooth coarse routes are sufficient for the reduced element; molecular smoothness and chemistry require further specification. The element has an allowed extension range covering the compact aperture interval. Chemical contour length, atom maps, and actual tether stiffness are additional realization data; no particular oligomer is inferred from this routing argument.

4.2 One energy for mechanics and binding

Write $s \in \{0, T, C\}$ for an empty site, target occupancy, and competitor occupancy. Let $r \in \{0,1\}$ be a local programming label distinct from the inherited stacking-edge labels. Set

$$b_0 = 0, \quad b_T = b_C = 4, \quad K = 16, \tag{10}$$

with contact energies

$$E_0 = 0, \qquad E_C = 10, \qquad E_T(r) = 10 + 6r. \tag{11}$$

The contact difference has the following specified electromechanical interpretation. Let the effective local field be $\mathcal{E}_r = 6re_2$, let the target's effective dipole be $d_T = e_2$, and let $d_C = 0$. Give both occupied states the common contact score 10, and include the coupling $-d_s \cdot \mathcal{E}_r$ in their energies. Then $E_T(r) = 10 + d_T \cdot \mathcal{E}_r$ and $E_C = 10 + d_C \cdot \mathcal{E}_r$ are exactly (11). Thus registry changes an explicit interaction channel, while the neutral competitor does not respond to that channel. The field map is constitutive data of the reduced model, not a consequence of a binary label alone. A molecular electrostatic realization must supply its charge, dielectric, screening, and contact-position data.

The control $c \in [3, 5]$ sets the rest aperture of the compliant element. Define

$$U_s(a; c, r) = \frac{K}{2}(a - c)^2 + b_s a - E_s(r), \qquad a \in [2, 6]. \quad (12)$$

The $b_s a$ term couples occupancy to the same aperture that determines the geometry. Occupancy thus changes the mechanical minimizer; binding is not merely attached as an unrelated output label.

Proposition 4.2 (Stable branch and admissible motion)**.** *For each s, c, r, the energy (12) has a unique minimizer*

$$a_s(c) = c - \frac{b_s}{K}. \quad (13)$$

Its second derivative is $K = 16$. All these minimizers lie in $[11/4, 5] \subset (2, 6)$. Every continuous control path in $[3, 5]$ produces a continuous equilibrium branch with the core and substrate clearances of Proposition 4.1. For fixed occupancy and control, the dissipative equation

$$\dot{a} = -\gamma\, \partial_a U_s(a; c, r), \qquad \gamma > 0, \quad (14)$$

has the solution

$$a(t) = a_s(c) + (a(0) - a_s(c))e^{-\gamma K t}.$$

It preserves $[2, 6]$ and converges to the unique minimizer.

Proof. Completing the square gives

$$U_s(a; c, r) = \frac{K}{2}(a - a_s(c))^2 + F_s(c, r), \quad (15)$$

$$F_s(c, r) = b_s c - E_s(r) - \frac{b_s^2}{2K}. \quad (16)$$

The minimizers are interior, so the constrained and unconstrained minima agree. The explicit solution is a convex combination of the initial aperture and its minimizer. The branch is affine in c and the clearance bounds are uniform on the larger interval $[2, 6]$. □

Changes of occupancy need not produce jumps in the physical aperture. If $s(t)$ and $c(t)$ are piecewise constant with finitely many switches on bounded time intervals, use (14) between switches and retain a continuously at each switch. The same invariant interval follows by concatenation. This supplies an admissible mechanical response, while the occupancy transition law and its timescale remain separate data.

The rigid-block idealization eliminates internal degrees of freedom. A local compliant-block extension may add regular internal coordinates ξ and the energy $\frac{1}{2}\xi^{\mathsf{T}} H \xi$ with a specified positive-definite H. These coordinates may include allowed stacking separation, slip, and twist deviations. At $\xi = 0$ the constructed branch is unchanged and its transverse Hessian is H. By continuity and the positive clearance margin, a sufficiently small coordinate neighborhood preserves core exclusion. This is a local harmonic constitutive extension; it does not assert that unparameterized π-stacking has the required stiffness.

4.3 A finite minimized-basin occupancy law

We now declare the thermodynamic reduction used for this witness. Each relaxed occupancy basin has effective energy F_s from (16). With unit target and competitor activities and inverse temperature one, assign

$$p_s(c, r) = \frac{e^{-F_s(c,r)}}{\sum_{u \in \{0,T,C\}} e^{-F_u(c,r)}}. \quad (17)$$

This finite minimized-basin law is part of the reduced model. It is not claimed to equal the exact continuous Gibbs integral of (12) on the bounded aperture interval. A physical free-energy reduction can add vibrational, solvation, and basin-volume terms; the robustness statement below permits bounded corrections.

Theorem 4.3 (A nonvacuous capture–release witness)**.** *The geometry (9), energy (12), and finite law (17) have the following properties:*

(i) At $r = 1, c = 3$, the target occupancy satisfies $p_T > 98/100$.

(ii) At $r = 1, c = 5$, the empty occupancy satisfies $p_0 > 97/100$.

(iii) At either control value, target-to-competitor occupancy odds are e^6 for $r = 1$ and 1 for $r = 0$.

(iv) For every $c \in [3, 5]$, $p_T(c, 1) > p_T(c, 0)$.

(v) Both endpoint settings are connected by the admissible branches of Proposition 4.2.

The numerical values are approximately $p_T(3, 1) = 0.9865944$ and $p_0(5, 1) = 0.9706172$.

Proof. The occupied basin energies are

$$F_T(c, r) = 4c - 10 - 6r - \tfrac{1}{2}, \qquad F_C(c) = 4c - 10 - \tfrac{1}{2},$$

and $F_0 = 0$. Thus

$$p_T(3,1) = \frac{e^{9/2}}{1 + e^{9/2} + e^{-3/2}},$$
$$p_0(5,1) = \frac{1}{1 + e^{-7/2} + e^{-19/2}}.$$

The positive-term exponential series gives

$$e^{9/2} > 80, \quad e^{3/2} > 4, \quad e^{7/2} > 33, \quad e^{19/2} > 10000.$$

For example partial sums through orders $7, 3, 9, 11$, respectively, already exceed these rational bounds. Consequently

$$p_T(3,1) > \frac{80}{80 + 1 + 1/4} = \frac{64}{65} > \frac{98}{100},$$

and

$$e^{-7/2} + e^{-19/2} < \frac{1}{33} + \frac{1}{10000} < \frac{3}{97},$$

which gives $p_0(5,1) > 97/100$. Taking the ratio of the occupied weights proves (iii). For fixed c the denominator of p_T is the target weight plus the same positive quantity $1 + e^{-F_C}$ in both registry settings. The target weight is strictly larger at $r = 1$, proving (iv). Part (v) is the established continuous branch construction. □

These statements describe selective equilibrium capture and a setting favorable to release. They do not specify the elapsed time to capture or release. A kinetic realization must add rates or barrier data compatible with the same basin energies. Likewise, the control changes the energy and is not cost-free: along a differentiable fixed-occupancy trajectory,

$$\frac{dU_s}{dt} = -\gamma(\partial_a U_s)^2 - K(a - c)\dot{c}. \tag{18}$$

The second term is the power supplied through the control coordinate. Occupancy or registry jumps have additional energy exchanges with their specified reservoirs. No autonomous pumping claim is contained in Theorem 4.3.

Corollary 4.4 (Open parameter family)**.** *The witness belongs to a nonempty open family of reduced models with strict target capture above* 98/100*, empty release above* 97/100*, a strict registry contrast at the endpoint settings, positive aperture stiffness, and interior equilibrium branches connecting the controls. The family may include small continuous changes of activities, contact energies, b_s, K, and sufficiently small smooth energy perturbations on the compact aperture–control domain. Geometric openness is relative to continuous, endpoint-compatible realizations of the fixed typed incidence, with uniform displacement over the compact aperture interval. Attachment sleeves and exits are retained or continuously transported compatibly. Sufficiently small perturbations preserve the positive core, corridor, and exterior connector margins.*

Proof. At the displayed parameters all performance inequalities are strict, the aperture Hessian is 16, and the branches remain at distance at least $3/4$ from the aperture boundary. Small C^2 energy perturbations preserve strict convexity; the implicit-function theorem gives unique nearby stationary branches, uniformly over the compact control interval. Their critical values and the finite occupancy probabilities vary continuously. The finitely many endpoint inequalities therefore persist on a common parameter neighborhood. Positive geometric separation persists under sufficiently small uniform displacement of the corresponding occupied sets and exterior routes, within the stated endpoint-compatible class. For the registry contrast along the entire control interval, its continuous positive difference attains a positive minimum by compactness, so it too persists under sufficiently small uniform perturbations. Thus the common neighborhood is nonempty and open in the stated finite-parameter and function-space topology. □

The construction proves existence and robustness for an explicitly declared reduced realization. Its next refinement is quantitative identification of the connector, stacking, dielectric, and transition-barrier parameters for a named substituted-chrysene assembly. The theorem does not require that refinement to be silently assumed completed.

5 Binding kinetics and controlled operation

5.1 A reversible finite binding law

Let $\mathcal{S} = \{0, T, C\}$ denote an empty site, target occupancy, and competitor occupancy. For a fixed registry and control, let $F_0 = 0, F_T, F_C$ be the minimized levels of the gate construction. With dimensionless activities $z_T, z_C > 0$ and inverse temperature $\beta > 0$, put

$$w_s = z_s e^{-\beta F_s}, \qquad Z = 1 + w_T + w_C,$$
$$(\pi_0, \pi_T, \pi_C) = Z^{-1}(1, w_T, w_C). \tag{19}$$

This is a declared finite basin model. The levels F_s are the mechanical minima, not asserted to be exact potentials of mean force obtained by integrating all molecular coordinates. Entropic basin corrections may be included as additional calibrated terms; the robustness result applies to sufficiently small corrections.

Definition 5.1 (Vacancy-mediated kinetics)**.** For an attempt frequency $\nu > 0$, define a generator Q by

$$q_{0s} = \nu \frac{w_s}{1 + w_s}, \quad q_{s0} = \nu \frac{1}{1 + w_s}, \qquad s \in \{T, C\}, \tag{20}$$

$$q_{TC} = q_{CT} = 0, \qquad q_{ii} = -\sum_{j \neq i} q_{ij}. \tag{21}$$

No transition changes the bound species without passing through the empty state. Activities represent exchange with specified substrate reservoirs.

Proposition 5.2 (Balance, dwell times, and relaxation)**.** *The law* (19) *is the unique stationary law of Q. The mean residence time of a bound species s before departure is $(1 + w_s)/\nu$. There exists $\gamma > 0$ such that every initial law p satisfies*

$$\|pe^{tQ} - \pi\|_{\mathrm{TV}} \leq \frac{1}{2} e^{-\gamma t} \left(\sum_{i \in \mathcal{S}} \frac{(p_i - \pi_i)^2}{\pi_i} \right)^{1/2}. \tag{22}$$

Proof. Every displayed off-diagonal edge rate is positive and the star graph is connected. Direct substitution gives $\pi_0 q_{0s} = \pi_s q_{s0}$. For a real function f on $\mathcal{S}$,

$$-\langle f, Qf \rangle_\pi = \tfrac{1}{2} \sum_{i,j} \pi_i q_{ij} (f_j - f_i)^2.$$

This form vanishes exactly on constants. The restriction of the self-adjoint operator $-Q$ to the finite-dimensional π-mean-zero space therefore has a strictly positive smallest eigenvalue γ. Spectral expansion gives contraction by $e^{-\gamma t}$ in $L^2(\pi)$. Apply it to the initial density p_i/π_i, using reversibility, and then use Cauchy–Schwarz to obtain (22). Irreducibility and the same kernel calculation give uniqueness. A bound state has only one exit, of rate q_{s0}, so its holding time is exponential with the stated mean. □

Remark 5.3 (Rate information is additional)**.** The common energy fixes the ratios $q_{0s}/q_{s0} = w_s$. It does not fix ν, nor does local detailed balance determine the individual kinetic barriers. Equation (20) supplies one admissible kinetic completion. A molecular application must replace or calibrate that completion through transition-state, mobility, or measured rate information. Equilibrium selectivity alone does not establish rapid capture.

5.2 A finite controlled execution

A control protocol must specify more than two favorable equilibrium laws. In the following reduced operational completion, occupancy transitions use a binary availability multiplier $\lambda(t) \in \{0, 1\}$: their active generator is $\lambda(t)Q$. The setting $\lambda = 0$ freezes occupancy during mechanical transfer. This is an explicit ideal gating control, not a consequence of the registry alphabet. The completion also includes occupancy-resolved sensing and event-triggered actuator commands; it is not an autonomous unsensed source.

For fixed occupancy s, write $b_0 = 0$ and $b_T = b_C = 4$. The scalar mechanical law is

$$\dot{a} = -\mu(16(a - c) + b_s), \qquad \mu > 0. \tag{23}$$

The polynomial energy is extended without change to transfer controls $c \in [21/8, 43/8]$. The interval $[3, 5]$ restricts the operating equilibria, not every transient command. The larger interval contains $[11/4, 21/4]$ with margin $1/8$, sufficient for the path lifts below at long enough durations. The actuator supplies the work recorded by the energy identity. In this hybrid completion controls are piecewise C^1, with instantaneous rest-control resets allowed at the finitely many event times on each finite active dwell. The aperture is continuous at such a reset. At fixed occupancy and aperture its work is

$$W_{\mathrm{reset}} = U_s(a; c^+, r) - U_s(a; c^-, r). \tag{24}$$

The continuous power identity holds between resets, and these work increments are added at resets. An occupancy jump is accounted for separately through its declared reservoir exchange. For example, after a jump $s \to s'$ at operating control c_* and aperture $a_s(c_*)$, the zero-velocity start of a new lift uses $c^+ = a_s(c_*) + b_{s'}/16$, which need not equal c_*. The specified reset, rather than an unaccounted smooth-control assumption, implements that change.

Lemma 5.4 (Controlled path lifting)**.** *Let $a_-, a_+ \in [11/4, 5]$. For fixed s, there is a smooth finite-time control taking* (23) *exactly from a_- to a_+, with aperture remaining in that interval and zero endpoint velocity. Its control values lie arbitrarily close to $[a_- + b_s/16, a_+ + b_s/16]$, interpreted as the interval between its endpoints, by increasing its duration.*

Proof. Choose a smooth monotone interpolation $a(t) = a_- + (a_+ - a_-)\chi(t/\tau)$ with $\chi(0) = 0$, $\chi(1) = 1$ and zero endpoint derivatives. Set

$$c(t) = a(t) + \frac{b_s}{16} + \frac{\dot{a}(t)}{16\mu}.$$

Substitution verifies the equation exactly. The correction is uniformly $O(\tau^{-1})$, while monotonicity gives the aperture bound. All paths stay in the positive-clearance domain of the gate. □

The finite occupancy model treats each state as a relaxed basin. A jump between basins can be implemented at the level of admissible paths by freezing the new species and inserting the preceding mechanical lift between the old and new aperture minima. This insertion changes physical elapsed time; it is not a derivation of the finite generator from an unreduced molecular diffusion. Define active kinetic time by $\theta(t) = \int_0^t \lambda(v)\, dv$. During active dwell the control is restored to its fixed operating setting, so the finite generator is the stated fixed Q on that clock. Dwell

lengths and Markov checkpoints below refer to this clock. During every inserted mechanical transfer $\lambda = 0$, so the active clock is paused. Binding/unbinding additionally uses the prescribed substrate corridor and reservoir interface. The ideal completion assigns a uniformly bounded duration to every complete paused event-handling stage, including any specified corridor transfer and settling; instantaneous interface updates are allowed as zero-duration cases. Those handling stages introduce no unmodelled occupancy changes.

Proposition 5.5 (Capture–release execution in the gated completion)**.** *For the explicit registry-*1 *witness, suppose the ideal occupancy hold, occupancy-resolved sensing, piecewise-smooth/reset actuator, and uniformly bounded complete reservoir/transfer interfaces just specified are available. Then finite active capture and release dwell lengths and a mechanically admissible transfer can be chosen so that the probability of target occupancy at the first checkpoint and an empty site at the second exceeds* 0.95*. The physical elapsed time is almost surely finite and has finite expectation. On successful release the construction can return to the original empty-site aperture without consuming the rigid scaffold.*

Proof. At capture control $c = 3$, the witness has $\pi_T > 0.98$; at release control $c = 5$, it has $\pi_0 > 0.97$. Since the state space is finite and all stationary masses are positive, the prefactor in (22) has a finite maximum over initial laws. Choose each dwell long enough to give total-variation error less than 10^{-4}. Freeze occupancy during the intervening mechanical path lift and insert the appropriate basin relaxation paths. Conditional on any state at the start of the release dwell, its final empty probability is greater than 0.9699. Consequently the desired joint event has probability greater than

$$(0.98 - 10^{-4})(0.97 - 10^{-4}) > 0.95.$$

If the release checkpoint is empty, the same mechanical lift returns its aperture to 3. The core graphs, port labels, and rigid-block membership are unchanged by these operations. For total active dwell T, the exit rates are at most 2ν, so the number of occupancy events is dominated by a Poisson variable of mean $2\nu T$. There are only finitely many endpoint pairs for the inserted paths; select their finite durations, and let $\tau_{\max}$ bound the complete per-event handling, including the other paused interfaces by hypothesis. Physical elapsed time is bounded by $T + \tau_{\max} N$ plus the fixed transfer and reset durations, and is therefore finite almost surely and in expectation. No claim of a successful return on every stochastic trajectory is needed; the asserted event has the displayed probability. □

Remark 5.6 (Open-cycle accounting)**.** The operation exchanges target and competitor molecules with reservoirs and uses actuator work. It establishes neither autonomous control nor positive net mechanical work from a single equilibrium bath. Repetition requires renewed reservoir conditions, admissible drive, and preservation of connector integrity. A failed release can be assigned a retry transition only with its own time and resource account.

5.3 Obstructions and source equivalence

Proposition 5.7 (Symmetry and equilibrium obstructions)**.** *Let two finite continuous-time Markov models, compared at a common clock, be related by a state bijection g preserving the initial law, controls, generator, and readout, in the sense that these data are transported by g. They have identical readout path laws. In a stationary reversible model, each oriented edge has zero net probability current.*

Proof. Conjugating the generator by the permutation of g conjugates its matrix exponential. Transition probabilities at any finite sequence of observation times are therefore transported by g. The preserved readout gives equal joint output distributions. For the second assertion, the current is $J_{ij} = \pi_i q_{ij} - \pi_j q_{ji} = 0$ by detailed balance. □

For physical-time hybrid models the equivalence data must also transport the pause-duration rules, reset maps, and controlled mechanical trajectories. Equality of active-time generators alone does not establish equality at physical observation times.

Registry changes can thus be observable only through some changed physical coupling, preparation, control, or readout. In the witness, the prescribed dipole–field projection is precisely such a changed coupling. Conversely, an endogenous and an engineered preparation that supply the same initial law and subsequent controlled dynamics have the same operational law [Sch26d]. Source provenance does not enter the generator as an additional force.

6 Interstitial function and molecular information

6.1 A moving interstitial domain

Let q be an admissible mechanical configuration and $\mathcal{B}(q)$ the union of its core, connector, and other excluded bodies. For a prescribed container $\Omega \subset \mathbb{R}^3$ and substrate radius $\rho > 0$, define

$$\mathcal{I}_\rho(q) = \{x \in \Omega : \operatorname{dist}(x, \mathcal{B}(q)) > \rho\}. \tag{25}$$

The relevant cavity is a specified component or labelled subregion of this accessible set, not necessarily the entire complement.

A contact field $\phi(q, x)$ and boundary labels give the interstice its chemical interpretation. Different readouts may distinguish cavities even when their unlabeled shapes are congruent.

Proposition 6.1 (Retention tube under deformation)**.** *Suppose $q : [0,1] \to \mathcal{Q}$ is continuous, its excluded bodies are nonempty compact sets, and a substrate-center path $x : [0,1] \to \Omega$ satisfies*

$$\inf_{t\in[0,1]} \operatorname{dist}(x(t), \mathcal{B}(q(t))) \geq \rho + \delta, \qquad \delta > 0.$$

If the center path is perturbed uniformly by less than $\delta/3$ and the excluded bodies uniformly in Hausdorff distance by less than $\delta/3$, and the perturbed centers remain in Ω, the perturbed center path remains accessible with clearance greater than $\delta/3$ beyond its radius.

Proof. For nonempty compact sets A, B, the distance functions satisfy $|\operatorname{dist}(x, A) - \operatorname{dist}(y, B)| \leq \|x - y\| + d_H(A, B)$. Apply this at each time and subtract the two perturbation bounds. □

This result concerns geometric retention or passage, not chemical binding. A tether that retains a peptide must be included in $\mathcal{B}$ and in its interface state. For the explicit gate, the moving center $x = (6 + a/2, 2, 2)$ follows an accessible path as a varies, so the tube condition has a positive witness. Post-release stability of a peptide requires its own interaction model after the relevant contacts have been removed.

6.2 Coupled code–product formation

Definition 6.2 (Joint production interface)**.** A joint production state consists of a current atom-and-bond graph, atom-origin labels, unused resource packets, charge/proton/electron accounts, a resident carrier, a variable coding register c, and a product record p. A certified production transition supplies a complete input and output state, its full read set and guard, a guarded transformation, and an admissible path or declared reaction law. Certification for a composed execution additionally checks the guard in the actual assembled current state, with every required fresh input and unused resource packet supplied. A decoding map d assigns products to coding records in its stated domain. The code–product invariant is $d(c) = p$.

The resident poly-adenosine scaffold and the variable coding register are different typed objects [Sch26c]. Coupled production may establish both records in one controlled process without asserting one elementary chemical event. To claim simultaneous amino-acid and codon formation at molecular resolution, the joint transition must include both product graphs and their shared atom/resource accounts.

Proposition 6.3 (Compatible extension of a code–product pair)**.** *Let $d(c) = p$, and let a certified transition add a coding segment b and a residue record a so that the declared extended decoder obeys $d(cb) = pa$. If each transition preserves the declared conserved accounts and the current output interface equals the next transition's input on shared coordinates, and every remaining input and guard is certified in the assembled current state, a finite sequence of such transitions preserves code–product correspondence and all declared conserved accounts.*

Proof. The base state satisfies the invariant. The stipulated decoder identity gives it after each extension. Interface equality identifies the shared current atoms and resources, while the separate input/guard certificate makes the next transition applicable without substituting an independent copy. Induction proves correspondence and preservation of each conserved account. This is a conditional composition theorem; existence of the chemical extension transitions is not a consequence of the decoder identity. □

6.3 Structure-first filtering and a coding lift

Let $\mathcal{P}$ be a finite set of peptide sequences and C a finite set of coding records. For each $p \in \mathcal{P}$, let Y_p be a specified nonempty finite collection of conformational states, or a finite discretization explicitly treated as the model itself. The candidate states form

$$\mathcal{Z} = \{(p, y) : p \in \mathcal{P},\ y \in Y_p\}.$$

A functional test $A(q, p, y) \in \{0, 1\}$ defines accepted states at the registry-generated environment q. Tests may encode backbone geometry, contact compatibility, or a named response observable. Calling a geometric pattern a helix or sheet does not alone identify a stable peptide basin.

Proposition 6.4 (Energy-gap filtering bound)**.** *Let $\mathcal{A} \subset \mathcal{Z}$ be a nonempty accepted set and let the law on $\mathcal{Z}$ be proportional to $\omega_z e^{-\beta G_z}$ with $\omega_z > 0$ and $\beta > 0$. Suppose*

$$G_a \leq E_* \ (a \in \mathcal{A}), \qquad G_b \geq E_* + \Delta \ (b \notin \mathcal{A}),$$

where $\Delta > 0$. Put $W_A = \sum_{a\in\mathcal{A}} \omega_a$ and $W_B = \sum_{b\notin\mathcal{A}} \omega_b$. Then

$$\Pr(\mathcal{Z} \setminus \mathcal{A}) \leq \frac{W_B e^{-\beta\Delta}}{W_A + W_B e^{-\beta\Delta}}. \tag{26}$$

Proof. The accepted partition sum is at least $W_A e^{-\beta E_*}$, and the rejected sum is at most $W_B e^{-\beta(E_*+\Delta)}$. The rejected probability is increasing in its own sum and decreasing in the accepted sum. Substitution yields (26). □

The factor W_B records competing multiplicity. Finite energy preference does not eliminate all rejected products at positive

temperature. Exact exclusion requires removal from admissible support, zero production weights, or a productive-release guard that actually forbids the unwanted outputs. The last alternative needs a realizable recognition mechanism; naming a guard is not its construction. Also, an equilibrium retention distribution does not by itself describe the distribution of a chemically synthesized product stream.

Proposition 6.5 (Finite coding section and its limitation)**.** *Let $d : C \to \mathcal{P}$ and let P_A be the sequence projection of the accepted states. If $P_A \subset d(C)$, there exists $e : P_A \to C$ with $d \circ e = \mathrm{id}_{P_A}$. If a fiber $d^{-1}(p)$ contains two distinct codes, no function of p alone recovers both possible historical codes.*

Proof. Order the finite set C and choose its first member in each nonempty fiber over P_A. This constructs e. For the second assertion, a function takes only one value at p, so it cannot equal two distinct historical values at that same input. □

A coding section is mathematical encodability. A reverse-recording machine additionally requires molecular recognition of the sequence, construction of a coding polymer, and a resource-accounted write operation. A conformational class generally determines neither a unique sequence nor a unique code. Article 99's selection within functional fibers is compatible with this multiplicity [Sch26d]; it does not supply the reverse-recording chemistry.

6.4 PCET as a specified mechanism

A PCET extension must identify donor and acceptor states, the proton pathway, electron/proton reservoirs, coupling coordinates, and energy changes. One may then ask whether the specified interaction changes a peptide nucleation barrier or stabilizes a conformational basin. Computations on lysine-containing helices show that an existing helical geometry can affect PCET [CLX+22]; that direction of dependence is not a proof that PCET in a chrysene pore produces a helix. Peptide-bond formation, nucleation, retention, and stability after release are distinct interfaces in the present framework.

7 An atlas of elementary machine realizations

Definition 7.1 (Realization chart)**.** A machine chart consists of a typed reference graph, a configuration domain, constitutive and reservoir data, allowed controls, an observable, and a proved operating specification. Charts with different bond graphs or internal state alphabets need not share a smooth manifold. Regular fixed-topology portions may have local manifold charts; topology-changing transitions are additional arrows between them.

The following entries define the scope of the series. Only the gate and the generic structural statements above are constructed here.

Hinge. Two stable subassemblies have a relative angular coordinate in an interval, with a specified pivot/attachment geometry. Its proof package comprises clearance, a restoring or control law, and a finite admissible motion. A freely rotating unstable fragment is not a controlled hinge.

Pore and recognition pocket. An accessible component of (25) has state-dependent transport or retention. A "ghost pocket," if used as terminology, denotes an explicitly specified transient contact pattern that need not persist in the empty state. Its existence is a configuration-and-interaction assertion, not a new molecular species by definition.

Slider. A relative translation is controlled while the remaining modes are stable. The explicit gate is a slider-type aperture realization. Its geometry is not relabelled a torsional hinge merely because both can open a cavity.

Rotor. A periodic coordinate has domain S^1. Existence of this coordinate is kinematic. A motor additionally requires directional current under a declared drive and a load/work balance. Detailed balance at stationarity obstructs a nonzero net cycle current.

Helicase-like assembly. Two coordinated gripping regions can be coupled to a displacement coordinate and a base-pair opening variable. Its operational specification must distinguish engagement, translocation, actual duplex separation, slippage, detachment, and reset. An eventual theorem should establish positive net unwinding under explicit drive and load conditions, not infer helicase function from a helical passage.

Proposition 7.2 (Finite execution composition)**.** *Suppose each stage has an admissible input/output state and execution, and the output of stage j equals the input of stage $j+1$ on shared molecular, resource, control, and environment coordinates. Suppose also that every remaining required input is supplied, every next-stage guard is satisfied in the assembled current state on its full read set, and no consumed resource is reused as fresh. If each stage preserves every invariant that remains active, their finite concatenation is an admissible execution preserving those invariants.*

Proof. Apply the first execution to its certified input. Interface equality identifies the shared input of the next execution; the

additional input and guard certificates supply its remaining prerequisites in that same assembled state. Induction establishes applicability and invariant preservation at every stage. Separate nonemptiness of unrelated stage spaces would not supply these equalities. □

This is the interface principle of the protocell construction [Sch26a], applied to machine charts. Material origins cannot be reused as unconsumed resources. A return to the original mechanical coordinate need not return reservoirs to their initial state. These distinctions allow the later series to investigate regenerative operation without treating a drawn cycle as proof of chemical closure.

8 Node-based computation and proof certificates

8.1 Molecular degrees of freedom and a numerical mesh

A discrete molecular solver begins with the physical degrees of freedom: core translations and rotations, connector coordinates, and selected charge or occupancy states. Each typed interaction contributes forces, torques, and tangent stiffness. Assembly of these contributions resembles a structural finite-element calculation, but a molecule is not merely a translational mesh point and an arbitrary interpolation edge is not a chemical bond.

An auxiliary mesh may approximate an electrostatic boundary-value problem, a solvent field, or a continuum deformation. Its interpolation functions and refinement index are separate data. Refining that numerical mesh, increasing the number of molecular nodes, and taking a homogenization limit are three distinct operations. No continuum limit or mesh-convergence theorem is assumed in the finite gate proof.

8.2 A finite-dimensional residual certificate

Proposition 8.1 (Certified local mechanical equilibrium)**.** *Let U be C^2 on a neighborhood of the closed Euclidean ball $\overline{B}(\widehat{y}, R)$ in a regular constrained coordinate chart. Suppose*

$$\nabla^2 U(y) \succeq mI \quad (y \in \overline{B}), \qquad m > 0,$$

and $r = \|\nabla U(\widehat{y})\| < mR$. Then there is exactly one stationary point y_* in the ball, it is interior, and

$$\|\widehat{y} - y_*\| \le r/m, \tag{27}$$

$$0 \le U(\widehat{y}) - U(y_*) \le r^2/(2m). \tag{28}$$

Proof. Continuity gives a minimum on the closed ball. At a boundary point y, integration of the Hessian along the radial segment gives

$$\nabla U(y) \cdot (y - \widehat{y}) \ge mR^2 - rR > 0.$$

An inward step decreases U, so a minimizer cannot lie on the boundary. Strict convexity gives uniqueness. Strong monotonicity applied to $\widehat{y}, y_*$ gives $m\|\widehat{y} - y_*\|^2 \le \nabla U(\widehat{y}) \cdot (\widehat{y} - y_*)$, proving (27). Strong convexity with base point $\widehat{y}$ bounds the energy gap by $rd - md^2/2$, where $d = \|\widehat{y} - y_*\|$; this expression is at most $r^2/(2m)$. □

A bound m requires more than a positive floating-point eigenvalue at one point. For example, a verified lower bound ℓ on the smallest eigenvalue of the computed central Hessian, a central matrix error at most ϵ_H, and a Hessian Lipschitz constant L_H imply

$$\nabla^2 U(y) \succeq (\ell - \epsilon_H - L_H R) I$$

throughout the ball. A positive right-hand side supplies a valid m. All coordinates must remain in the admissible chart, including excluded-volume margins and gauge conditions.

Proposition 8.2 (Sampled-path clearance certificate)**.** *Let $g : [0, 1] \to \mathbb{R}$ be an L-Lipschitz clearance function along a specified path. Suppose sample times include both endpoints and successive times differ by at most h. If every sample has $g(t_i) \ge \delta$, then $g(t) \ge \delta - Lh/2$ for all $t \in [0, 1]$.*

Proof. Every time lies within $h/2$ of a sampled endpoint of its containing interval. Apply the Lipschitz inequality. □

Thus sampled noncollision becomes a proof only after a suitable interpolation rule and a valid Lipschitz bound are supplied. A solver trace with positive sampled clearance alone does not exclude an intervening collision.

8.3 Reproducible witness checks

The explicit witness is analytic. Table 1 records selected values that can also be evaluated directly. Rounded probabilities are illustrations; the rational bounds in Theorem 4.3 provide the strict certificate. For parameter sweeps, useful negative controls are removal of the dipole–field contrast ($r = 0$), removal of the aperture-dependent binding term, loss of transverse stiffness, and violation of the control or collision constraints. A test must distinguish a changed physical model from a relabelling of the same one. The computational companion [Sch26f] records 472 passing deterministic checks under Python 3.12.14, NumPy 2.3.5, and SciPy 1.17.0. The count includes parameterized cases, not 472 separate theorems. Exact rational certificates, exact finite samples, floating-point checks, and an 81-point robustness grid are distinguished. Numerical tolerances are absolute and relative 2×10^{-11}; numerical eigenvalues are not presented as interval certificates.

Quantity	Value
Core count	16
In-plane edges (both blocks)	16
Stacking edges (both blocks)	8
Reference determinant	64
Aperture stiffness	16
Empty minima, capture/release	3, 5
Occupied minima, capture/release	2.75, 4.75
Target capture probability	0.9865944 . . .
Empty release probability	0.9706172 . . .
Target/competitor odds, $r = 1$	e^6

Table 1: Dimensionless reduced-model witness. The compliant interblock element is additional to the internal edge counts.

The formal companion [Sch26g] contains 47 theorem declarations successfully checked by Lean 4.24.0. Its generic algebraic results are over the rational numbers; reference geometry and finite arithmetic are checked by kernel reduction. No admitted proof, custom axiom, or native decision oracle is used. The scope is a structural and exact rational core, not a complete formalization of the manuscript's real analytic, continuous-geometric, stochastic, or chemical claims. The companions embed their full sources and provide separate execution records.

9 Discussion and conclusions

The fibrated architecture supplies a durable address system for a moving material. Its discrete base records where a component belongs in the reference construction; the physical embedding records where that component is now. This separation permits an assembly to retain molecular identity and typed connectivity while performing a nonperiodic deformation. It also prevents a numerical mesh from replacing the molecular specification it is intended to analyze.

The first existence result is deliberately elementary but joint. Sixteen labelled cores give two three-dimensional patches. Their oblique reference cell respects the axiomatic freedom from Cartesian orthogonality. A compliant aperture, an explicit dipole–field projection, and a binding-dependent mechanical term produce one common model. Its stable branches, functional inequalities, kinetic completion, and controlled execution have separate proofs that use the same state and energy data. Strict margins make the witness robust rather than a single equality-constrained design point.

The mathematical novelty of this construction is not a new general minimization theorem or a replacement for statistical mechanics. It is the explicit realization link between the finite chrysene architecture and an operational machine model, together with a precise accounting of which ingredients are inherited and which are constitutive. Standard compactness, implicit-function, and finite Markov arguments become useful only after that link has been specified. The witness's numerical constants demonstrate nonvacuity of the model class; they do not predict an experimental yield or a molecular binding energy.

A next-stage mechanical study should identify actual substituent and tether choices, measure or calculate stacking slip/twist stiffness, and replace the effective field projection by a dielectric and charge model. It should also test whether selective binding survives conformational entropy and whether the required kinetic barriers are compatible with the desired dwell times. If these refinements move the parameters outside the proved neighborhood, the existence certificate must be recomputed rather than retained by analogy.

For peptide organization, the interstitial domain becomes a bridge between structural mechanics and molecular information. One route co-produces a coding record and a residue/product record through compatible transformations. Another selects a suitable sequence/conformation class and then chooses a coding representation. The finite coding-section result clarifies that encodability need not mean historical-code recovery, while the leakage bound makes sequence multiplicity an explicit part of structural selection. Neither route is reduced to a geometrical name such as "helix" or "pocket."

The machine atlas consequently separates a realized gate from prospective hinges, driven rotors, and helicase-like composites. The latter require energy-transducing cycles and actual strand-separation laws. The appropriate synthesis of later papers will be a common realizability theorem across their interfaces, not the inference that independently possible modules must coexist. In that synthesis, endogenous and exogenous sources remain alternative preparation mechanisms whose operational comparison depends on the states, controls, and resources they actually supply.

In summary, the labelled reference architecture supplies the address and incidence system; a declared local program and constitutive interactions make its selected realization a controllable deformable material; controlled admissible deformation and substrate coupling make a selected region a machine. The present gate gives a complete reduced-model witness for this progression and a reusable proof architecture for its extension.

A Source concordance and realization levels

The following correspondence records the scope of inherited structures.

1. Revised axioms A1–A3 provide a labelled core, its symmetry distinctions, and ordered primary directions. They do not impose perpendicularity or a numerical transfer anisotropy.

2. A4–A6 provide directional bridge compatibility, exact reference closure, and the indexed three-dimensional network. The stacking-edge registry and the tensorial skeleton are

retained as distinct data. Physical π-stacking supplies a possible constitutive realization of the abstract interlayer relation.

3. A7–A9 provide the parent operation/observable and spectral framework. A finite machine uses finite observable assignments and explicitly defined mechanical operators; it is not asserted to satisfy the full infinite spectral construction unchanged.

4. A10–A11 provide separately specified transfer and response structures. Configuration-dependent charge and polarization laws are additional couplings, not deductions from the indexing lattice.

5. A12 provides an admissibility language. A permitted symbolic edge, a continuous path, and a dynamically driven transition remain different certificates.

6. The metamaterial study motivates lateral connection, stacked integration, and interstitial function. Its architectural proposal is not used to infer a global physical free-energy minimum or exact orthogonal locking without a constitutive proof.

7. The finite-ICL pilot supplies earlier component templates and a common functional model. This article refines that program by linking a finite geometry to one explicit energy and binding construction.

B Exact bounds and a verification recipe

For $x > 0$ define $S_N(x) = \sum_{j=0}^{N} x^j/j!$. All summands are positive, so $e^x > S_N(x)$. The inequalities used in the gate proof reduce to the four rational comparisons

$$S_7(9/2) > 80, \quad S_3(3/2) > 4,$$

$$S_9(7/2) > 33, \quad S_{11}(19/2) > 10000.$$

They may be checked by common denominators or exact rational arithmetic. The release comparison additionally uses

$$\frac{1}{33} + \frac{1}{10000} < \frac{3}{97},$$

and the capture comparison uses $64/65 > 49/50$. These exact checks separate the theorem from rounded tabular values.

For reproduction of the probability table, use $K = 16$, $b_0 = 0$, $b_T = b_C = 4$, $E_0 = 0$, $E_C = 10$, and $E_T = 10 + 6r$. Compute $F_s = b_s c - E_s - b_s^2/(2K)$ and normalize $\exp(-F_s)$ over $s = 0, T, C$. All activities and inverse temperature are one in that table. This recipe does not require the molecular coordinates to be rescaled to any particular physical unit.

C Proof coverage

The analytic results in this manuscript cover the declared finite structural, constrained mechanical, occupancy, and interface models. The sixteen-core example certifies the nondimensional reduced gate; the rate completion certifies a reversible finite kinetic model; the gated execution additionally assumes ideal occupancy hold and actuator availability. The peptide statements certify filtering and coding relations under their stated hypotheses, not chemical synthesis. The atlas records unproved extension targets separately from the constructed gate. The delivered Python and Lean companions [Sch26f, Sch26g] have been executed and compiled respectively. The Python suite checks finite instances and exact arithmetic; the Lean module checks the specifically listed structural and rational statements, including square completion, rational minimum uniqueness, finite coding representatives, occupancy sufficient conditions, and resetwork algebra. Real exponentials, the general implicit-function and compactness arguments, continuous exterior routing, spectral mixing, clock changes, and chemical realization are not machine-checked by that module. Compiling either companion in Overleaf typesets its source listing; it does not run the embedded Python or Lean program. No experimentally calibrated machine performance is claimed.

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