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APEPM: Geometry-Based Pre-Screening for Bond Feasibility and Orbital Participation

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Overview

Armstrong's Probabilistic Electron Phase-Space Overlap Model (APEPM) is a closed-form, wavefunction-free geometric framework for determining whether a chemical bond is *geometrically feasible* and which atomic orbital regions must participate if bonding occurs. APEPM is designed to operate as a fast pre-screening and constraint layer prior to quantum-mechanical (QM), density functional theory (DFT), or machine-learned electronic structure methods.

Problem Addressed

High-throughput molecular, materials, and biomolecular workflows routinely evaluate candidate geometries that are electronically or geometrically incompatible with bonding. These failures are often detected only after expensive QM or surrogate calculations, consuming computational resources without yielding physically meaningful results.

A fast, interpretable **geometric precondition** for bond feasibility can eliminate invalid candidates early, reduce downstream compute load, and provide structural context for later electronic analysis.

What APEPM Does

APEPM determines whether mandatory electron cloud overlap exists between bonded atoms using closed-form geometry derived from effective electron cloud radii and bond length. When overlap exists, the model computes:

- Overlap radius, area, and volume (shared electron phase-space)
- Which atomic orbital regions geometrically intersect this shared region
- Admissible probability bounds for participating orbital regions

All quantities are analytic, geometry-driven, and explicitly independent of wavefunctions, basis sets, coordinate grids, or energy minimization.

Intended Role in Computational Pipelines

APEPM is not an electronic structure method and is **not intended to replace QM or DFT**. Instead, it functions as a fast screening and interpretive layer upstream of those methods.

Typical usage pattern:

Candidate geometry
↓
APEPM geometric screening
↓
Reject infeasible bonds / rank by overlap depth
↓
QM / DFT / ML electronic structure
↓
Property evaluation

APEPM can be used to:

- Reject geometries with zero electron cloud overlap
- Rank candidates by degree of geometric bonding feasibility
- Identify orbital regions that must participate geometrically
- Provide interpretable geometric context for downstream calculations

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Performance Characteristics

APEPM evaluations scale linearly with bond count and execute in milliseconds even for large biomolecules, on consumer hardware. No numerical convergence, grids, or iterative solvers are required.

What APEPM Explicitly Does *Not* Do

APEPM does not compute or approximate:

- Electronic energies
- Electron density distributions
- Charge transfer or polarization magnitude
- Reaction barriers or spectroscopic observables

Orbital “participation” refers strictly to **geometric inclusion** in shared electron phase-space, not energetic contribution or chemical dominance.

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