Archaea and Computational Simulations Refute the RNA World Hypothesis, Strongly Confirm the Matter World Hypothesis

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Abstract
The RNA World Hypothesis (RWH), which posits RNA as the sole primordial molecule driving life's origin, faces significant challenges due to RNA's chemical instability, limited catalytic capacity, and inability to form stable protocells. In contrast, the Matter World Hypothesis (MWH) proposes that life emerged from synergistic interactions among RNA, DNA, peptides, lipids, and mineral catalysts in prebiotic environments. This article integrates molecular dynamics (MD) and dissipative particle dynamics (DPD) simulations with biological evidence from Archaea—Earth's most ancient lifeforms—to refute RWH and validate MWH. Simulations show RNA-only systems degrade rapidly (25–35% RMSD in 100 ns), exhibit poor catalysis (k_{cat} ~0.003–0.006 min^{-1}), and form unstable vesicles (lipid order ~0.45, lifetime ~10–15 hr). MWH systems achieve high stability (<10% RMSD), robust catalysis (k_{cat} ~0.058–0.068 min^{-1}), and stable vesicles (lipid order ~0.65, lifetime ~40–50 hr). Archaeal biology, including DNA-based replication and peptide-driven metabolism, supports MWH's synergistic framework. These findings necessitate a paradigm shift in origins-of-life research, with implications for astrobiology and synthetic biology.

Keywords: Abiogenesis, RNA World Hypothesis, Matter World Hypothesis, Archaea, Molecular Dynamics, Dissipative Particle Dynamics, Protocells, Prebiotic Chemistry, Astrobiology

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1. Introduction

The RNA World Hypothesis (RWH), proposed by Gilbert (1986), suggests that RNA's dual role as genetic material and catalyst enabled life's emergence. However, RNA's susceptibility to reactive oxygen species (ROS), poor catalytic efficiency, and inability to sustain stable protocells undermine its plausibility. The Matter World Hypothesis (MWH), advanced by Hashemi (2025a, 2025b), argues that life arose from a cooperative network of RNA, DNA, peptides, lipids, mineral catalysts (e.g., montmorillonite, Zn^{2+}), and energy sources like pyrophosphate (PPi) in prebiotic environments such as hydrothermal vents, ice, tidal pools, and wet-dry cycles.

This study employs molecular dynamics (MD) simulations with the CHARMM36 force field to model molecular interactions and dissipative particle dynamics (DPD) to capture lipid vesicle dynamics, as described by Groot and Warren (1997). These simulations compare RNA-only, ribosome-only, ribosome-peptide, and MWH-based protocells under prebiotic conditions, incorporating ROS-induced damage and vesicle metrics (formation, fusion, stability). Biological evidence from Archaea, which thrive in extreme environments resembling early Earth, provides further support. This article synthesizes computational and archaeal evidence to refute RWH and establish MWH as the leading model for life's origin.

2. Limitations of the RNA World Hypothesis

The RWH is undermined by critical flaws, as evidenced by computational simulations and archaeal biology.

2.1 Chemical Instability of RNA

RNA's fragility in prebiotic conditions limits its role as the sole primordial molecule. MD simulations reveal that RNA-only systems degrade rapidly, with a 25–35% increase in root-mean-square deviation (RMSD) within 100 ns, driven by ROS-induced damage (e.g., 8-oxo-guanine formation, k_{ROS} ~0.01–0.03 ns^{-1}) (Hashemi, 2025b). Hydrothermal vents (80 ± 15°C, ROS 0.45 ± 0.18 mM) cause the most severe degradation (35% RMSD), while ice environments (-5 ± 3°C) show slightly less damage (25% RMSD). Mutation rates are high (4.5–5.0 × 10^{-7} per nucleotide), with 10–15% of bases forming 8-oxo-guanine.

Archaeal evidence corroborates these findings. Hyperthermophilic Archaea, such as *Pyrococcus furiosus*, thrive at 100°C using DNA as their primary genetic material. RNA's half-life at such temperatures is mere minutes, making it unsuitable as a stable genetic repository in early Earth's harsh conditions.

2.2 Limited Catalytic Efficiency

Ribozymes, central to RWH, exhibit poor catalytic performance. MD simulations show peptide bond formation rates (k_{cat}) of 0.003–0.006 min^{-1} in RNA-only systems, 94–97% lower than MWH systems (Hashemi, 2025b). Ribosome-only systems perform worse (k_{cat} ~0.001–0.003 min^{-1}), while ribosome-peptide systems improve slightly (k_{cat} ~0.008–0.014 min^{-1}) but remain 80–86% less efficient than MWH.

Archaea rely on metalloproteins, such as [NiFe]-hydrogenases, for metabolic processes like methanogenesis, rather than RNA-based catalysis. This suggests that peptides and metal catalysts were critical for early metabolism, challenging RWH's reliance on ribozymes.

2.3 Unstable Protocells

DPD simulations, which model vesicle dynamics at a mesoscopic scale (Groot & Warren, 1997), reveal that RNA-only vesicles are prone to rupture, with a lipid order parameter of ~0.45, an area per lipid of ~0.75 nm^2, and a lifetime of 10–15 hours. Ribosome-only vesicles are similarly unstable (lipid order ~0.40, lifetime ~8–12 hr). These systems fail to maintain structural integrity under prebiotic stresses.

In contrast, Archaea utilize stable, ether-linked lipids (e.g., glycerol dialkyl glycerol tetraethers, GDGT), which self-assemble without RNA involvement. Their membranes exhibit a higher lipid order parameter (~0.65), reflecting the robustness required for early protocells.

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3. The Matter World Hypothesis: A Synergistic Framework

The MWH posits that life emerged from cooperative interactions among RNA, DNA, peptides, lipids, and catalysts. Computational and archaeal evidence strongly supports this model.

3.1 Computational Validation

MD and DPD simulations demonstrate MWH's superiority (Hashemi, 2025a, 2025b):

- **Structural Stability**: MWH systems show minimal degradation (<10% RMSD increase in 100 ns), even in harsh environments like hydrothermal vents.
- **Catalytic Efficiency**: Peptide bond formation rates reach k_{cat} ~0.058–0.068 min^{-1}, driven by Zn^{2+} (0.06 mM), PPi (0.15 mM, ΔG ~–7 kcal/mol), and ribosome-peptide interactions. Binding energies (ΔG ~–7 to –9 kcal/mol) indicate strong molecular synergy.
- **Vesicle Stability**: DPD-modeled vesicles (80% oleate/decanoate) achieve a lipid order parameter of ~0.65, an area per lipid of ~0.62 nm^2, and a lifetime of 40–50 hours, with rare fusion or rupture events.
- **Mutation Rates**: RNA mutation rates are lower (2.3×10^{-7} per nucleotide), and DNA's presence reduces rates further (1.1×10^{-8} per nucleotide), with only 2–5% 8-oxo-guanine formation.

Statistical analyses confirm these results. ANOVA ($p < 0.001$, F = 1200–2800) and Cohen's d (0.8–1.2 for MWH vs. 0.1–0.5 for RNA-only) highlight significant differences. Regression models (R^2 = 0.50–0.82) identify RNA integrity, DNA presence, ROS levels, and vesicle stability as key predictors. Correlations (e.g., catalysis vs. ROS, r = –0.65 to –0.85; vesicle stability vs. mutation rate, r = 0.60 to 0.75) underscore MWH's robustness.

3.2 Archaeal Corroboration

Archaea provide a biological analog for MWH:

- **Genetic Systems**: Archaea use DNA and protein-based polymerases (e.g., PolB) for replication, not RNA self-replicators, contradicting RWH's core premise.
- **Metabolism**: Energy pathways, such as methanogenesis, rely on Fe-S clusters and peptides, not RNA. PPi, not ATP, serves as the ancestral energy currency, aligning with MWH's simulated use of PPi.
- **Membranes**: Ether-linked lipids self-assemble without RNA catalysis, forming stable membranes that withstand extreme conditions, consistent with DPD results.

3.3 Prebiotic Chemistry

Mineral surfaces like montmorillonite (1.2 g/L in simulations) catalyze peptide-RNA-lipid co-assembly, enhancing stability and function (Hashemi, 2025b). Hybrid RNA-peptide oligomers, modeled as proto-ribosomes, outperform pure RNA systems, with binding energies (ΔG ~–7 to –9 kcal/mol) indicating strong interactions. These findings align with experimental studies on mineral-driven polymerization in prebiotic settings.

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4. Implications

The combined evidence necessitates a shift from RWH to MWH in origins-of-life research.

4.1 Revising Abiogenesis Models

Textbooks and research frameworks should adopt MWH's synergistic model, emphasizing the co-evolution of RNA, DNA, peptides, lipids, and catalysts. Experimentalists should focus on replicating MWH systems using microfluidics, cryo-EM, or multi-scale simulations (e.g., DPD/MD/QMMM).

4.2 Astrobiology Applications

Life-detection missions to Mars, Europa, or Enceladus should target multi-molecular signatures (e.g., lipids, metals, polymers) rather than RNA alone. Simulations suggest ice environments stabilize minimal systems, while tidal pools support complex protocells, guiding mission design (Hashemi, 2025a).

4.3 Synthetic Biology

Engineering artificial cells requires integrating RNA, peptides, and lipids from the outset, with DPD-guided vesicle design informing minimal cell construction (Groot & Warren, 1997).

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5. Discussion

MD and DPD simulations reveal that RNA-only and ribosome-only systems collapse due to ROS-induced damage, poor catalysis, and unstable vesicles (Hashemi, 2025b). Ribosome-peptide systems show marginal improvements but remain inferior to MWH, which achieves robust stability, catalysis, and vesicle dynamics across diverse environments. Ice environments favor minimal systems, while tidal pools support complex protocells, reflecting MWH's adaptability. These findings align with prior agent-based modeling, which showed synergistic systems persisting up to 780,000 steps versus RNA-only systems collapsing within 20,000–60,000 steps (Hashemi, 2025a).

RWH proponents might argue that specific microenvironments could stabilize RNA, but the consistent instability across simulated conditions weakens this claim. MWH's complexity requires further study to elucidate the sequential or parallel emergence of its components. Future work should validate these findings experimentally and explore multi-scale modeling.

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6. Conclusion

Molecular dynamics and dissipative particle dynamics simulations, coupled with archaeal biology, conclusively refute the RNA World Hypothesis. RNA's chemical instability, limited catalytic efficiency, and unstable vesicles render it an implausible sole driver of life's origin. The Matter World Hypothesis, supported by robust computational metrics (<10% RMSD, k_{cat} ~0.058–0.068 min^{-1}, vesicle lifetime ~40–50 hr) and archaeal evidence (DNA-based replication, peptide-driven metabolism, stable ether lipids), provides a compelling synergistic model. This paradigm shift redefines abiogenesis, offering new directions for astrobiology, synthetic biology, and the search for life beyond Earth.

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