

TDG/TQ Pre-Data Predictions for Supercooled Ion-Doped Water Clusters

Derived Directly from the Proton Curvature Threshold (No Molecular Fitting)

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November 12, 2025

Abstract

This record provides pre-data predictions from the Time-Dilation Geometry / Timeless Quanta (TDG/TQ) framework for observables expected in supercooled, ion-doped water cluster experiments at the November 2025 ACS Physical Chemistry Division sessions. All scaling relations originate solely from the proton curvature lock-in developed in *Timeless Quanta* [1]. No experimental molecular parameters, force-field coefficients, or fitted potentials are used. A three-shell TDG/TQ curvature potential yields an H₂O dimer O–O separation of **2.910 AA** (exp: 2.80 AA; deviation 3.9%). Predictions for RDF contraction, THz-band coherence, and dopant-induced Mpemba acceleration follow directly from the same geometry. Full Python code is provided for transparency and reproducibility.

1 Lock-In Geometry: The Proton as the Universal Curvature Anchor

In the TDG/TQ framework, all mass-energy arises from curvature exceeding the critical threshold Θ_c within radius r_c :

$$r_c = 0.447 fm, \quad \Theta_c = 1.62 \times 10^{38} m^{-2}, \quad K = -1.93 \times 10^{47}. \quad (1)$$

This collapse radius acts as the universal scale from which curvature shells, Ricci gradients, and hybrid (Gaussian–exponential) profiles arise. In TDG/TQ, this geometric threshold—not quantum fields—governs the structure of quanta and all emergent bound states. Molecular predictions follow from scaling these curvature tails outward from the nuclear domain.

2 Three-Shell Curvature Model of the Water Dimer

The O–O dimer is ideal for testing geometric scaling because hydrogen bonding is dominated by a single intermolecular coordinate. TDG/TQ models the interaction using three effective curvature shells:

1. Core curvature at the donor oxygen ($d_1 = 0$).
2. Core curvature at the acceptor oxygen ($d_2 = R$).
3. Bridge curvature centered at the H-bond midpoint ($d_3 = R/2$).

Note. A simpler one-shell TDG/TQ model (treating each oxygen as isolated) predicts an O–O minimum of 3.118AA. The three-shell model’s improved agreement (2.910 AA vs. 3.118 AA) demonstrates that proper geometric coupling pulls the prediction toward experiment *without parameter adjustment*.

2.1 Flux-Conserving Exponential Tails

TDG/TQ requires curvature flux to be conserved as shells expand:

$$\lambda_i^2 d_i = \lambda_{\text{nuc}}^2 r_c, \quad (2)$$

giving

$$\lambda_i = \lambda_{\text{nuc}} \sqrt{\frac{r_c}{\max(d_i, r_c)}}, \quad \lambda_{\text{nuc}} = \frac{1}{2r_c}. \quad (3)$$

2.2 Gaussian Confinement

The Gaussian confinement term reflects molecular-scale delocalization:

$$\sigma_{\text{eff}} = 1.4AA. \quad (4)$$

2.3 Effective Potential

The TDG/TQ curvature potential is

$$V(R) = \sum_{i=1}^3 -\exp[-\lambda_i |R - d_i|] + \frac{R^2}{2\sigma_{\text{eff}}^2}. \quad (5)$$

3 Prediction: O–O Minimum at 2.910 Å

Numerical minimization (Sec. 4) yields:

Predicted O–O separation	2.910 Å
Experimental reference	2.80 Å
Deviation	3.92%

This result is parameter-free: only r_c , Θ_c , and λ_{nuc} determine the geometry.

4 Reproducible TDG/TQ Code

```
1 import numpy as np
2 from scipy.optimize import minimize_scalar
3 import matplotlib.pyplot as plt
4
5 # =====
6 # TDG/TQ FIXED CONSTANTS (LOCKED)
7 # =====
8 r_c = 0.447e-15
9 sigma_nuc = 0.81e-15
10 lambda_nuc = 1.12e15
11 m_p = 1.67e-27
12
13 # Small epsilon to avoid singularities
14 eps = 1e-20
15
16 # =====
17 # H2O GEOMETRY (no fitting)
18 # =====
19 d_OH = 0.96e-10
20 angle_° = 104.5
```

```

21 angle_rad = np.°2rad(angle_°)
22
23 O_A = np.array([0.0, 0.0, 0.0])
24 H1_A = np.array([d_OH, 0.0, 0.0])
25 H2_A = np.array([d_OH*np.cos(angle_rad),
26                 d_OH*np.sin(angle_rad), 0.0])
27
28 def place_monomer_B(R):
29     O_B = np.array([R, 0.0, 0.0])
30     H1_B = O_B + np.array([d_OH, 0.0, 0.0])
31     H2_B = O_B + np.array([d_OH*np.cos(angle_rad),
32                             d_OH*np.sin(angle_rad), 0.0])
33     return O_B, H1_B, H2_B
34
35 # =====
36 # TDG/TQ SCALING
37 # =====
38 def lambda_eff(distance):
39     d = max(distance, eps)
40     return lambda_nuc * np.sqrt(r_c / d)
41
42 sigma_eff = 1.4e-10
43
44 # =====
45 # SHELL POTENTIAL
46 # =====
47 def V_shell(r, center):
48     d = np.linalg.norm(r - center)
49     d = max(d, eps)
50     lam = lambda_eff(d)
51     return -np.exp(-lam * d) + (d*d) / (2 * sigma_eff * sigma_eff)
52
53 # =====
54 # TOTAL MULTI-SHELL POTENTIAL
55 # =====
56 def V_total(R):
57     O_B, H1_B, H2_B = place_monomer_B(R)
58     centers = [O_A, H1_A, H2_A, O_B, H1_B, H2_B]
59
60     V = 0.0
61     for c in centers:
62         V += V_shell(O_A, c)
63         V += V_shell(H1_A, c)
64         V += V_shell(H2_A, c)
65         V += V_shell(O_B, c)
66         V += V_shell(H1_B, c)
67         V += V_shell(H2_B, c)
68     return V
69
70 # =====
71 # FIND MINIMUM ENERGY SEPARATION
72 # =====
73 res = minimize_scalar(V_total, bounds=(1e-10, 6e-10), method='bounded')
74 R_min_A = res.x * 1e10
75
76 print("===== TDG/TQ RESULT =====")
77 print("Predicted O-O separation:", R_min_A, "A")
78 print("Reference (exp): 2.80 A")

```

```

79 print("Deviation:", abs(R_min_A - 2.80)/2.80 * 100, "%")
80 print("=====")
81
82 # =====
83 # PLOT
84 # =====
85 R_range = np.linspace(1e-10, 6e-10, 600)
86 V_range = [V_total(R) for R in R_range]
87
88 plt.figure(figsize=(10,6))
89 plt.plot(R_range*1e10, V_range)
90 plt.axvline(R_min_A, color='r', linestyle='--')
91 plt.axvline(2.80, color='g', linestyle='--')
92 plt.xlabel("O-O Separation (Å)")
93 plt.ylabel("V_eff (arb units)")
94 plt.title("TDG/TQ H2O Dimer Potential (No Fitting)")
95 plt.grid(alpha=0.3)
96 plt.tight_layout()
97 plt.show()

```

Listing 1: TDG/TQ 3-shell H2O dimer prediction (2.910 Å).

5 Predictions for Supercooled Ion-Doped Water Clusters

Applying TDG/TQ’s \sqrt{N} curvature-amplification rule and exponential-tail deformation yields:

Observable	Baseline	TDG/TQ Prediction	Prediction	Falsification Threshold
Mpemba acceleration (NaCl, MgCl ₂ , CsI)	≤ 8% (MD)	10–15% relaxation	faster re-	< 8% or no dopant dependence
THz coherence shoulder	Absent in MD	0.75–1.05 THz; lifetime 40–90 ps		No shoulder or lifetime < 20 ps
RDF O–O contraction (quench)	2–3% MD scatter	0.6–1.4% contraction	contrac-	Outside 0.6–1.4%

6 Genuine Prediction: CsI-Doped RDF Second Peak

For CsI-doped supercooled water clusters ($N=20$ molecules, $T=190$ K, 10 K/min quench), TDG/TQ predicts contraction of the second RDF peak (H–O ≈ 0.96 Å) by $\Delta r/r = 1.1\%$ (band 0.9–1.3%) vs. classical MD baseline 0.2–0.4%. Derivation: $\Delta r/r = \sqrt{N}\delta\kappa/\ln(\alpha N)$, with $\delta\kappa = 0.04$, $\alpha = 6 \times 10^5$, $N=20 \rightarrow 1.1\%$. Falsify: < 0.7% or no dopant dependence.

7 Falsifiability Criteria

- O–O prediction falsified if $|R - 2.80 \text{ Å}| > 0.20 \text{ Å}$.
- Mpemba acceleration falsified if < 8% or no dopant dependence.
- THz shoulder falsified if no 0.75–1.05 THz band appears.
- RDF contraction falsified outside 0.6–1.4%.

8 Acknowledgments

Artificial intelligence tools (Claude, Grok, ChatGPT) were used for code debugging and LaTeX formatting. All physical reasoning, derivations, and scientific claims are the author's work.

9 References

References

- [1] J. Rouse, *Timeless Quanta: A Threshold Geometry for Mass, Entropy, and Time*, Zenodo (2025). DOI: 10.5281/zenodo.17329617.