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Unusual Melting Behavior of Nitrogen at Extreme Pressures from Large-Scale Machine-Learned Potential Simulations

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Abstract

The phase diagram of nitrogen under extreme conditions is crucial for elucidating pressure-induced polymerization and designing novel high-energy-density materials, yet its melting behavior remains controversial. Resolving this debate has been challenging, because obtaining a reliable melting curve requires equilibration of both solid and liquid phases over large system sizes that exceed what standard first-principles simulations can afford computationally. In this work, we develop a machine-learned potential trained to SCAN meta-GGA accuracy to perform large-scale molecular dynamics simulations lasting several nanoseconds. We report an unusual melting curve with a cg-N/molecular-liquid/polymeric-liquid triple point at 104 GPa, which marks the onset of a plateau. These behaviors arise from the solid polymerizing before the liquid under compression, a process we term asynchronous polymerization. Furthermore, the melting-curve plateau coincides with the onset of optical reflection in dynamic laser-heating experiments. This correspondence corroborates the simulation prediction and provides a microstructural explanation for the optical signal by identifying it with the melting of cg-N into a metallic polymeric fluid. By reconstructing nitrogen's high-pressure phase diagram and clarifying its unusual melting behavior, this work provides a theoretical benchmark for high-pressure melting in simple molecular systems.

1 Introduction

Pressure-driven bond reconstruction in light-element systems is a central problem in high-pressure physics, and elemental nitrogen provides a prototypical molecular model for exploring it[1, 2]. Over a wide pressure range, the strong $N \equiv N$ triple bond keeps nitrogen molecular, yet compression gradually enhances intermolecular interactions[3–6]. Once intermolecular interactions become comparable to intramolecular forces, the triple bonds dissociate, inducing a transition to a non-molecular, single-bond-dominated polymeric network[7–9]. This pressure-driven transition makes nitrogen a key model for high-energy-density materials and yields a highly complex phase diagram including unusual melting behavior[2, 10–16].

Early PBE-based first-principles simulations and concurrent optical and Raman experiments all supported the presence of a melting maximum, although the reported maxima differ significantly, ranging from 50 to 88 GPa[13–17]. However, the latest synchrotron X-ray diffraction (XRD) experiments observed a monotonically increasing melting temperature up to 120 GPa[18], directly contradicting the existence of such a maximum. Moreover, early studies largely attributed this unusual melting behavior to a nearby first-order liquid-liquid phase transition (LLT)[14, 15, 17]. However, two independent Raman and XRD studies detected no trace of liquid polymeric nitrogen at the corresponding pressures[13, 16, 18]. The latest dynamic optical spectroscopy clearly indicates that substantial polymerization and metallization of fluid nitrogen are actually delayed until pressures exceed 125 GPa[19]. These significant discrepancies between theory and experiment, as well as among experiments themselves, highlight the limitations of current methods and hinder our understanding of high-pressure nitrogen, thereby motivating a more reliable approach to re-examine its phase diagram.

To bridge this gap, a recent study used the more accurate SCAN meta-GGA functional and pushed the stability boundary of liquid molecular nitrogen up by about 15 GPa[20]. However, the associated computational cost typically restricts the simulations to hundreds of atoms—a scale too small to avoid severe finite-size effects that strongly influence the predicted phase boundaries[14, 15]. To overcome these limitations, machine-learned potentials (MLPs) offer an ideal solution. By combining quantum-mechanical accuracy with classical-scale efficiency, MLPs enable the large-scale, long-time simulations necessary to determine the phase boundaries reliably[21–28]. Applying this approach to high-pressure nitrogen is expected to resolve the long-standing debates over its melting curve and the underlying physical mechanisms.

Here, we develop an MLP with SCAN meta-GGA accuracy (SCAN-MLP) to investigate the melting behavior of nitrogen under extreme pressures via large-scale two-phase molecular dynamics (MD) simulations. These simulations employ supercells containing $\sim 5,000$ atoms and are performed over timescales ranging from hundreds of picoseconds to 10 ns, thereby reaching size and time scales far beyond those accessible to direct ab initio MD simulations. We find an unusual melting curve: a sharp rise near 82 GPa is followed by a plateau above 104 GPa, where cg-N, molecular liquid, and polymeric liquid meet at a triple point. We attribute this behavior to asynchronous polymerization: the solid polymerizes into cg-N first under compression, while the molecular liquid undergoes a transition to a polymeric liquid only at higher pressures. Moreover, this plateau coincides with the onset of optical reflection in dynamic laser-heating experiments, which we attribute to the melting of cg-N into a metallic polymeric fluid. We further locate a first-order liquid-liquid phase transition terminating at a critical point (98 GPa, 3500 K). These results resolve long-standing controversies and establish a theoretical benchmark for nitrogen’s high-pressure phase diagram.

2 Results and Discussion

2.1 Melting Curve

We first employed the trained SCAN-MLP to simulate the melting curve of molecular solid nitrogen (δ -N₂). We find that the melting temperature T_m increases monotonically with pressure (blue solid circles in Fig. 1), whereas the melting-line slope dT_m/dP progressively decreases (tangents drawn at the melting points). Within this investigated pressure range, our melting line is consistent with the melting boundaries determined by in situ Raman[13, 16] (open pentagons and open triangles in Fig. 1) and synchrotron X-ray diffraction[18] (gray solid line in Fig. 1), and it also agrees with the melting line obtained by Donadio et al. from PBE-GGA-based thermodynamic integration[15] (gray dashed line in Fig. 1). This agreement across distinct experimental techniques

and theoretical approaches verifies the reliability and accuracy of the MLP-based large-scale two-phase simulations used in this work. We then extended the melting-curve calculations to higher

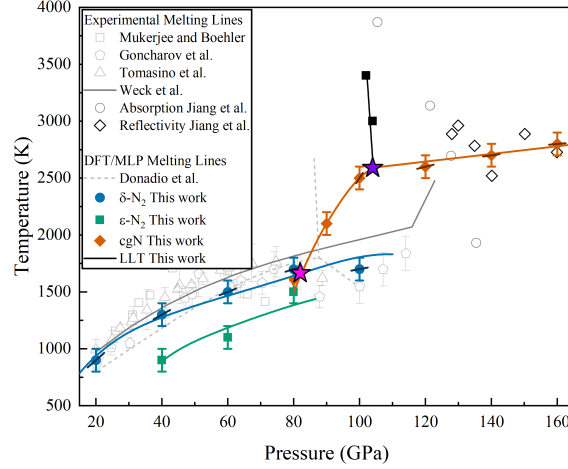


Fig. 1 Nitrogen melting lines. Experimental: Mukherjee[17] (squares), Goncharov[13] (pentagons), Tomasino[16] (triangles), Weck’s melting line[18] (dark-gray curve), and onsets of absorptive (circles) and reflective (diamonds) fluid states[19]. Donadio’s DFT line is dashed[15]. This work shows δ -N₂ (blue circles), ϵ -N₂ (green squares), and cg-N (orange diamonds) melting points; dark-blue/dark-orange tangents give Clausius–Clapeyron slopes; error bars span two-phase MD bracketing intervals. Magenta and purple stars mark the δ -N₂/cg-N/liquid and cg-N/molecular-liquid/polymeric-liquid triple points.

pressures. At ~ 82 GPa, the gradually flattening δ -N₂ melting line intersects the rapidly rising melting line of cubic-gauche polymeric nitrogen (cg-N). At the intersection, the coexisting liquid is still composed primarily of N₂ molecules. This intersection, located at ~ 82 GPa and 1700 K, marks a triple point (magenta star in Fig. 1) where molecular solid (δ -N₂), polymeric solid (cg-N), and the molecular liquid coexist. Upon further compression, the melting curve—corresponding to the cg-N/molecular-liquid coexistence line—rises rapidly.

The predicted triple point and the overall trend of the melting curve, which exhibits a gentle increase below the triple point and a steep rise above it, are qualitatively consistent with the synchrotron XRD measurements reported by Weck et al.[18] (dark-gray solid line in Fig. 1), whereas they disagree with the melting-temperature maximum and the subsequent negative slope predicted by earlier PBE-based first-principles calculations[15] (gray dashed line in Fig. 1). This discrepancy arises from our use of the SCAN meta-GGA functional[29], which more accurately captures van der Waals interactions and thereby raises the stability pressure of the molecular liquid[20], together with the inclusion of ϵ -N₂ and cg-N as additional solid reference phases beyond the single δ -N₂ phase considered in Ref.[15], resulting in a more comprehensive melting curve.

To further justify using δ -N₂ as the molecular-solid reference in our thermodynamic comparisons, we also computed the ϵ -N₂ melting curve over 40–80 GPa and found it to be consistently lower than the δ -N₂ curve. This indicates that δ -N₂ is thermodynamically favored over ϵ -N₂ near melting in this pressure range (i.e., at the δ -liquid coexistence, $G_\delta \approx G_{\text{liquid}} < G_\epsilon$), confirming that δ -N₂ is an appropriate molecular-solid reference phase in this work.

Upon further compression to ~ 104 GPa, the cg-N melting line intersects the liquid–liquid transition (LLT) boundary. Thus, (~ 104 GPa, ~ 2590 K) can be identified as a cg-N/molecular-liquid/polymeric-liquid triple point (the purple star in Fig. 1), which terminates the LLT line, unlike the solid–solid–liquid triple point at ~ 82 GPa. At still higher pressures, the melting curve progressively flattens and eventually levels off into a plateau. This behavior is further corroborated by the high-reflectivity transition boundary reported by Jiang et al.[19] (black open diamonds in Fig. 1), obtained from pulsed-laser-heated diamond anvil cell experiments with in situ optical characterization.

To provide a rigorous thermodynamic explanation for the unusual evolution of the melting curve, we decoupled the contributions of the enthalpy (ΔH) and volume (ΔV) changes across the phase boundaries based on the Clausius–Clapeyron relation (Fig. 2a-c). Below 82 GPa, ΔH remains within 0.034–0.036 eV/atom and ΔV within 0.016–0.017 Å³/atom, with the melting slope staying low, such that the melting temperature rises slowly with pressure. Upon pressurization to ~ 82 GPa, the cg-N phase replaces molecular δ -N₂ as the reference solid phase along the melting curve.

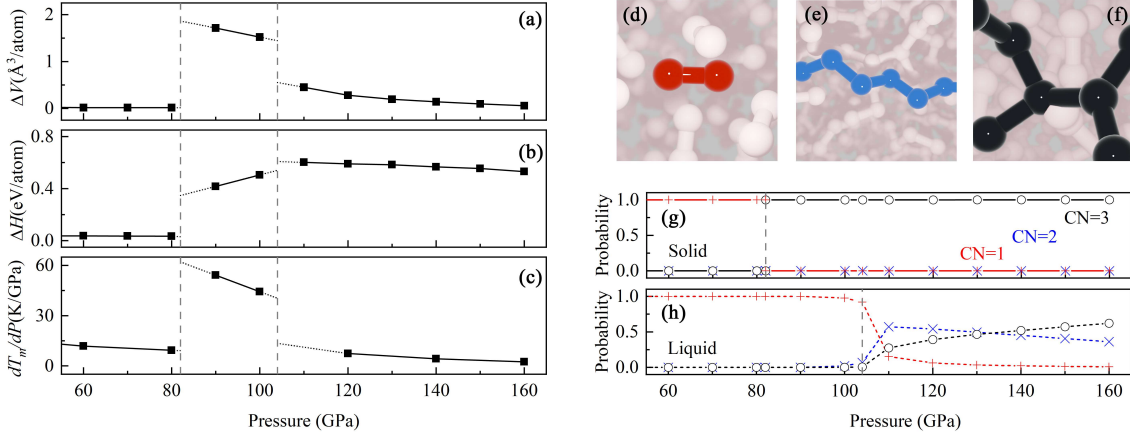


Fig. 2 Thermodynamic and structural origins of unusual melting behavior of nitrogen. (a) Volume difference between the liquid and solid phases near the melting point, ΔV . (b) Enthalpy difference between the liquid and solid phases near the melting point, ΔH . (c) Slope of the cg-N melting curve, dT_m/dP , evaluated from the Clausius–Clapeyron relation. (d–f) Schematics of the local atomic configurations associated with coordination numbers of (d) CN = 1 (molecular), (e) CN = 2 (chain-like), and (f) CN = 3 (network-like). (g, h) Evolution of the CN fractions with pressure in the solid (g, solid lines) and liquid (h, dashed lines) phases, with red, blue, and black curves representing CN = 1, 2, and 3, respectively.

Across this transition, ΔH increases by a factor of ~ 11 , while ΔV increases by a factor of ~ 141 , a much more pronounced rise. Since the increase in ΔV greatly exceeds that of ΔH , the melting slope jumps abruptly to about 60 K/GPa, and the melting curve rises steeply with pressure. With further compression to ~ 104 GPa, the liquid phase undergoes a first-order liquid-liquid transition from a molecular liquid to a denser polymeric liquid. During this transition, ΔH decreases by only $\sim 11\%$, whereas ΔV drops sharply by $\sim 62\%$. As the decrease in ΔV substantially exceeds that of ΔH , the melting slope drops sharply to about 13 K/GPa, and the melting curve flattens. Under continued compression, ΔH remains nearly unchanged while ΔV continues to approach zero, driving the melting slope toward zero as well, so that the melting curve enters a plateau region. Overall, the unusual evolution of the melting curve is dictated predominantly by the anomalous variations in ΔV , while ΔH plays only a secondary role.

To further elucidate the microscopic origin of such anomalous ΔV behavior, we analyzed the coordination-number distribution $P(\text{CN})$ for molecular (CN=1), chain-like (CN=2), and network-like (CN=3) environments in both phases (Fig. 2d–h). Below 82 GPa, both the solid and liquid phases are dominated by one-coordinated molecular structures, leading to similar local environments and a small solid–liquid volume difference. Above 82 GPa, the liquid retains its one-coordinated molecular character, whereas the solid phase switches to the denser cg-N phase, which is dominated by three-coordinated network structures. The resulting pronounced disparity in local structure substantially enlarges the solid–liquid volume difference. At ~ 104 GPa, the liquid undergoes a first-order liquid–liquid transition from molecular to polymeric nitrogen, accompanied by a rapid decrease in the one-coordinated fraction and a sharp increase in the two- and three-coordinated fractions. Upon further compression, the three-coordinated (network-like) fraction continues to grow while the two-coordinated (chain-like) fraction decreases, indicating that the local structure of the polymeric liquid progressively approaches that of the cg-N solid. Consequently, the solid–liquid volume difference diminishes and the melting curve enters a plateau regime. In summary, the anomalous melting behavior originates from the asynchronous polymerization of the solid and liquid phases: the solid polymerizes first at ~ 82 GPa, creating a large local-structural disparity (and thus large ΔV), while the subsequent polymerization of the liquid above ~ 104 GPa restores local-structural similarity, driving both ΔV and the melting slope toward zero.

2.2 Electronic properties

The plateau region of our melting curve (beyond ~ 104 GPa) shows good agreement with the temperature range of the reflective states observed by Jiang et al.[19], suggesting that the onset of the reflective states is closely linked to the melting process. To elucidate the relationship between melting and the emergence of the reflective states at the microscopic level, we combined electronic density of states (DOS) analysis with systematic calculations of the frequency-dependent optical

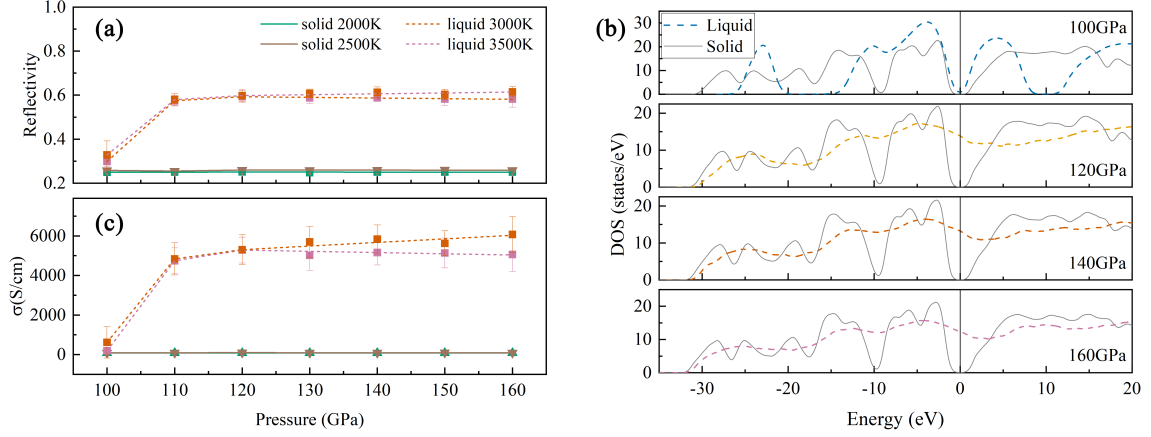


Fig. 3 Pressure dependence of the optical and electronic transport properties of nitrogen, together with the evolution of its electronic structure. (a) Optical reflectivity at 1064 nm and (c) electrical conductivity of solid cg-N and liquid nitrogen plotted against pressure for several temperatures. (b) Electronic density of states of solid cg-N at 2500 K and of liquid nitrogen at 3000 K at representative pressures; the Fermi level is set to zero.

conductivity $\sigma(\omega)$ of solid (cg-N) and liquid nitrogen over 100–160 GPa using the Kubo–Greenwood formalism[30, 31], from which both the optical reflectivity and the direct-current (DC) conductivity were derived.

Fig. 3a shows the pressure dependence of the reflectivity of nitrogen in different phases at an incident wavelength of 1064 nm. The reflectivity of solid cg-N remains nearly constant at ~ 0.26 throughout the entire pressure range. By contrast, the molecular liquid at 100 GPa exhibits a reflectivity only slightly higher than that of the solid; as pressure increases and the molecular liquid transforms into a polymeric liquid, the reflectivity rises steeply to ~ 0.6 , in agreement with previous first-principles predictions[32]. This abrupt rise in reflectivity corresponds to the system entering the polymeric liquid phase, which can be reached either via dissociation of the molecular liquid or via melting of solid cg-N.

To clarify the electronic-structure origin underlying this optical transition, we further examined the evolution of the DOS. As shown in Fig. 3b, at 100 GPa both solid cg-N and molecular liquid nitrogen exhibit a pronounced gap near the Fermi level (E_F), indicative of nonmetallic behavior. Upon further compression, the band gap of solid cg-N remains essentially unchanged, whereas the molecular liquid dissociates and polymerizes, causing the gap to close completely and producing a finite DOS across E_F , characteristic of a metallic electronic structure.

To corroborate the metallic character at the macroscopic transport level, we computed the DC electrical conductivity of the system (Fig. 3c). Solid cg-N exhibits an extremely low conductivity (only about 80–90 S/cm) that is insensitive to temperature and pressure, consistent with its stable semiconducting nature. Molecular liquid nitrogen at 100 GPa likewise shows low conductivity. However, once the system crosses the transition boundary into the polymeric liquid phase, the DC conductivity rises abruptly to $\sim 4800 - 6000$ S/cm, identifying it as a metallic liquid.

Furthermore, we calculated the frequency-dependent reflectivity spectrum of liquid nitrogen at 130 GPa and 3000 K (Fig. S3); its overall trend agrees with previous first-principles calculations[32] and the experimental data of Jiang et al.[19], further validating the quantitative reliability of the theoretical simulations and transport calculations performed in this work.

In summary, the simultaneous abrupt changes in optical reflectivity, electronic DOS, and DC conductivity are mutually consistent and align with the high-reflectivity and metallic character previously predicted for the polymeric liquid, thereby confirming that the reflective state corresponds to the metallic polymeric liquid phase of nitrogen.

2.3 Liquid-liquid transition

Next, we focus on the molecular-to-polymeric liquid-liquid phase transition (LLPT) in fluid nitrogen. To characterize this transition behavior, extensive canonical (NVT) molecular dynamics simulations driven by the SCAN-MLP were performed on a 1,728-atom supercell. These simulations systematically scanned a broad range of volumes along seven distinct isotherms from 2000 to 5000 K, yielding the isothermal pressure-volume (P-V) equations of state (EOS) presented in Fig. 4. In the high-temperature regime (3600–5000 K), these P-V isotherms decrease monotonically without any pressure drop, indicating the absence of macroscopic thermodynamic signatures

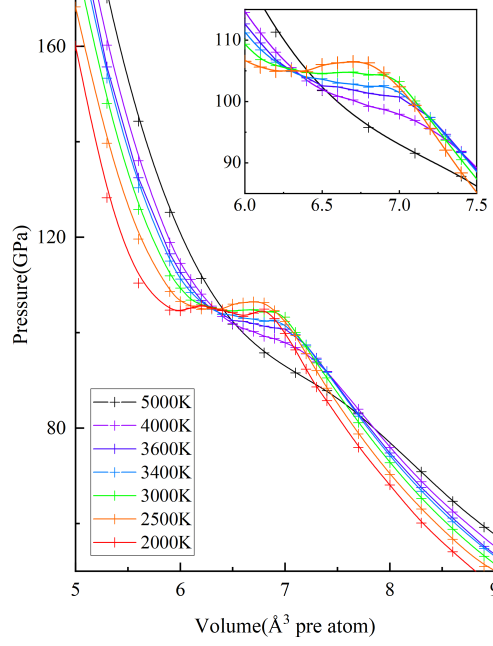


Fig. 4 Calculated equations of state for liquid nitrogen along various isotherms. Solid lines with different colors represent various temperatures. Inset: Enlarged view of the phase transition region.

for a first-order phase transition. Conversely, as the temperature decreases to the 2000–3400 K range, the isotherms begin to exhibit distinct non-monotonic regions. Within these regions, the mechanical stability condition, $(\partial P/\partial V)_T \leq 0$, is locally violated, resulting in the formation of classic van der Waals loops. Such loops serve as quintessential thermodynamic signatures of a discontinuous phase change, thereby confirming the occurrence of a first-order LLPT. Consequently, this molecular-to-polymeric transition is strictly confined to the lower-temperature regime, which directly implies that its associated critical point (CP) must lie at the boundary between these two distinct topological behaviors: between 3400 and 3600 K.

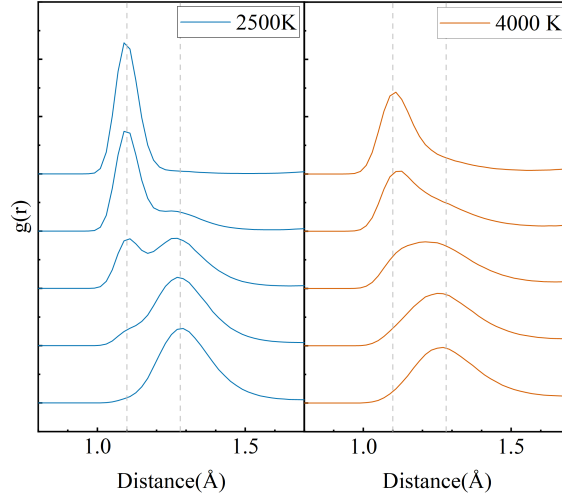


Fig. 5 Pair distribution functions, $g(r)$, of fluid nitrogen at varying densities during isothermal compression. The left and right panels correspond to the isotherms at $T = 2500$ K and 4000 K, respectively. From top to bottom, the simulated densities are 3.23, 3.47, 3.69, 3.94, and 4.15 g/cm³. Curves are vertically offset for clarity.

The microstructural evolution further corroborates this conclusion. Fig. 5 displays the pair distribution functions, $g(r)$, during isothermal compression at 2500 K (left) and 4000 K (right). At the 2500 K isotherm, for pressures $P < 104$ GPa, the qualitative shape of $g(r)$ remains largely unchanged, characterizing a molecular-dominated liquid; specifically, the first nearest-neighbor peak is located at 1.1 Å, corresponding to the equilibrium bond length of the $N \equiv N$ triple bond. Upon further compression to approximately 104 GPa, a second peak emerges at 1.28 Å,

marking the formation of polymeric single bonds. Within this pressure interval, the simultaneous presence of both the 1.1 Å and 1.28 Å peaks provides clear structural evidence for the two-phase coexistence of the molecular and polymeric fluids. As the pressure continues to rise above 110 GPa, the initial 1.1 Å peak completely vanishes, signifying the system’s thorough transformation into a non-molecular, purely polymeric phase. In contrast, at the higher temperature of 4000 K (Fig. 5, right), the first peak of $g(r)$ shifts continuously to 1.28 Å with increasing pressure. This continuous structural evolution (devoid of any bimodal coexistence regime) substantiates the deduction drawn from the equations of state: a first-order phase transition from a molecular to a polymeric liquid occurs in the low-temperature regime.

Combining the non-monotonic features of the EOS with the structural evolution of $g(r)$, we determine that the critical point (CP) of the LLPT in fluid nitrogen is located at approximately 98 GPa and 3500 K. The estimated CP, together with the established phase boundaries, is illustrated in the phase diagram in Fig. 6, where the previous findings are also included for comparison.

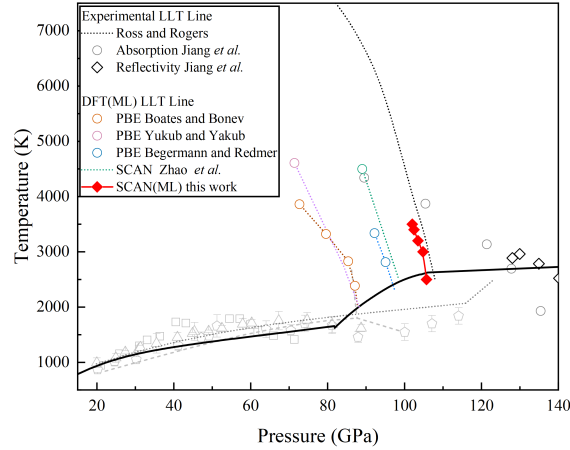


Fig. 6 Liquid-liquid phase boundary. The red solid line is this work’s liquid-liquid phase transition (LLPT); the black dashed line is Ross and Rogers’ chemical-model boundary[33]. PBE-based LLPTs are dashed in orange (Boates and Bonev[14]), purple (Yakub and Yakub[34]), cyan (Driver and Militzer[35]), blue (Bergermann and Redmer[36]); green dashed line is Zhao et al.’s SCAN meta-GGA LLPT[20]. Pink circles (diamonds) mark absorption (reflection) onsets in heated DAC experiments[19].

Our SCAN meta-GGA critical transition pressure lies above the PBE-based predictions. The physical origin of this pressure shift is rooted in the intrinsic capabilities of the functionals: compared to PBE, the SCAN meta-GGA functional more accurately captures both the strong intramolecular covalent bonds and the intermediate-range intermolecular interactions. This improved description effectively enhances the relative stability of the molecular liquid phase, thereby pushing the phase boundary toward higher pressures[20].

Regarding the critical temperature, our obtained value is lower than several earlier theoretical predictions. We attribute this discrepancy primarily to the large-scale supercell (1,728 atoms) employed in our work, a system size far exceeding the 64-atom limit of previous studies (Fig. S4). The vicinity of a phase transition critical point is typically characterized by pronounced long-wavelength fluctuations and severe finite-size effects. With a larger simulation system, these spatial fluctuations are more comprehensively accommodated, ultimately providing more robustly converged equations of state and more reliable critical parameters.

3 Conclusion

In summary, by employing large-scale molecular dynamics with a high-accuracy machine-learned potential trained on SCAN meta-GGA data, we have reconstructed a comprehensive and self-consistent high-pressure phase diagram of nitrogen. Our work resolves the long-standing controversy over nitrogen’s melting behavior, revealing that the unusual melting curve—featuring a steep rise followed by a prominent plateau—is governed by asynchronous polymerization, where the solid polymerizes before the liquid under compression. Furthermore, by directly linking the onset of optical reflection to the formation of the polymeric fluid, we provide a coherent atomistic interpretation of the experimentally reported high-reflectance states. This refined phase framework

not only revises earlier theoretical predictions to align with existing experimental measurements, but also serves as a reliable theoretical benchmark for exploring complex phase transitions in other compressed molecular systems.

4 Methods

4.1 Model

We built the SCAN-MLP using the DPA3 descriptor in Deepmd-kit 3.1.0[26, 37], which realizes a LiGS-based (line-graph-series) message-passing network. DPA3 maps the configuration to a first-order graph $G^{(1)}$ (atoms, nearest-neighbor bonds) and a second-order graph $G^{(2)}$ (bond angles). Atom features are updated from their connected bonds, and bond features from their two endpoint atoms. Residual connections link $G^{(1)}$ and $G^{(2)}$, capturing many-body interactions while preserving translational, rotational, and permutational invariance.

The network used 3 update layers and a maximum line-graph order of 2. In $G^{(1)}$, the atom and bond feature dimensions were 128 and 64 with a cutoff of 6.0 Å; in $G^{(2)}$, the angle feature dimension was 32 with a cutoff of 4.0 Å. The resulting invariant features were passed to a fitting network with 3 hidden layers of 240 neurons and residual connections, which output the total energy. The model was trained for 10^6 steps with dynamic loss weights: the energy weight was gradually increased from 0.2 to 20, the force weight decayed from 100 to 60, and the virial weight rose from 0.02 to 1. The learning rate was exponentially decayed every 5,000 steps, smoothly decreasing from 1.0×10^{-3} to 3.0×10^{-5} .

4.2 Training Data

A hierarchical strategy was used to construct a compact and high-quality training dataset for SCAN-MLP. First, large-scale NPT-AIMD simulations with the PBE functional[38] sampled a broad region of phase space, covering the solid phases δ -N₂, ϵ -N₂, and cg-N, as well as molecular and polymeric liquids, over pressures of 20–160 GPa and temperatures of 300–5000 K. This produced about one million configurations. Next, we applied farthest point sampling (FPS)[39] to extract 30,000 representative structures, reducing labeling cost while preserving configurational diversity. Finally, these 30,000 selected configurations were relabeled using the SCAN meta-GGA functional[29], yielding high accuracy energies and forces.

4.3 DFT

All DFT calculations and AIMD simulations were performed with VASP[40]. We used supercells of 128 atoms for δ -N₂, 192 atoms for ϵ -N₂, and 216 atoms for cg-N. In the initial phase-space exploration, each temperature–pressure point was simulated for 20,000 steps (20 ps in total), using PAW pseudopotentials[41, 42], the PBE functional[38], a 400 eV plane-wave cutoff, and Γ -point Brillouin zone sampling. For the subsequent high-accuracy relabeling, we switched to the SCAN meta-GGA functional[29] with an increased and converged plane-wave cutoff of 800 eV.

4.4 Electronic calculations

The static electronic structures were calculated with Quantum ESPRESSO[43, 44] for 15–20 equilibrium snapshots drawn from 64-atom SCAN-MLP MD trajectories, using the PBE-GGA functional[38] and norm-conserving pseudopotentials with five valence electrons ($2s^2 2p^3$), a 100 Ry plane-wave cutoff, a $4 \times 4 \times 4$ k-point mesh, and 600 bands, with Fermi-Dirac smearing set to the ionic temperature of the corresponding MD simulation.

From these electronic structures, the optical and electrical properties were obtained using the Kubo-Greenwood formalism[30, 31] as implemented in the KGEC package[45], which directly computes the real and imaginary parts of the complex conductivity tensor $\sigma(\omega)$, including an exact zero-frequency formulation for the DC conductivity σ_{DC} that avoids low-frequency singularities. In the Kubo-Greenwood evaluation, the Dirac δ function was broadened by a 0.2 eV Lorentzian. The complex dielectric function and reflectivity were subsequently derived from $\sigma(\omega)$. The full set of electrical and optical properties was computed individually for each snapshot, and the resulting quantities were then averaged over the ensemble to yield the reported values.

Data availability

The SCAN-MLP model developed in this study and the SCAN training dataset are publicly available in the Zenodo repository[46]. All other relevant numerical data supporting the findings of this study are available from the corresponding author upon reasonable request.

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Author contributions

Hanyu Liu, Yu Xie, and Xin Zhong designed the research. Jie Luo performed the computational simulations. Jie Luo, Yuan Ma, Chennan Song, and Hanyu Liu analyzed the data, and wrote and revised the manuscript.

Competing interests

The authors declare no competing interests.

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