

Structure of liquid mercury at high pressure

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The atomic-scale structure and melting curve of liquid mercury was measured using *in situ* synchrotron x-ray diffraction (SXRD) at pressure and temperature (p - T) conditions up to 9.44(2) GPa and 651(1) K. *Ab initio* molecular dynamics (AIMD) simulations were employed to obtain a detailed atomistic model of the liquid structure. The results reveal a pronounced flattening, and potential maximum, in the measured melting curve between 6 and 9 GPa. The structure factors $S_{\text{HgHg}}(Q)$ and pair distribution functions $g_{\text{HgHg}}(r)$ calculated from the AIMD simulations are in good overall agreement with the SXRD measurements under comparable reduced densities and temperatures, indicating that the atomistic structure of liquid Hg is well captured by AIMD. With increasing pressure, the principal peak in $S_{\text{HgHg}}(Q)$ shifts to higher Q , with the subsidiary peak at $Q = 2k_F$ experiencing a concomitant shift consistent with the increased electron density. Considering the Evans t -matrix formulation of the Ziman theory of liquid metals, the structural $S(2k_F)$ term is expected to have only a weak influence on the electrical resistivity under compression. In contrast, the pressure-induced broadening and shift of the d -projected density of states towards the Fermi level is consistent with enhanced near-resonant d -electron scattering, and a corresponding increase in resistivity, analogous to the behavior of first-row transition metals. Analysis of the measured $g_{\text{HgHg}}(r)$ functions, and AIMD trajectories in real space, indicates that the liquid structure experiences a progressive development towards simple hard-sphere-like behavior at increasing p - T along the melting curve. However, topological cluster classification analysis shows that while the structural fingerprint of liquid Hg strongly resembles an effective hard-sphere system, even at the highest pressures investigated it contains more many-body motifs than expected for this simple model.

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I. INTRODUCTION

Elemental liquid metals are often classified into three types based on their interatomic structure and macroscopic properties [1]. Type-I liquids, including most transition, alkali, alkaline earth, and rare-earth metals, are well described by models based on the strong short-range repulsion of ion cores arising from the collective delocalization of valence electrons, resulting in random, close packed structures analogous to hard spheres [2]. However, deviations from this idealized behavior can arise in systems where electrostatic interactions become

significant. For example, type-II liquid metals which include the group 12 elements zinc (Zn), cadmium (Cd), and mercury (Hg), exhibit slight distortions from hard-sphere behavior due to weakly directional bonding and partial d -electron localization. Type-III liquid metals, including gallium (Ga), silicon (Si), germanium (Ge), and tin (Sn), exhibit stronger deviations from hard-sphere behavior, forming complex structures with low local coordination numbers due to a competition between simple hard-sphere packing and topological ordering of short-range covalently bonded tetrahedral structures [3]. These liquids exhibit anomalous macroscopic properties, including volume contraction during melting associated with negative slopes and maxima in their high-pressure melting curves. This can be understood in terms of the Clausius-Clapeyron relation

$$\frac{dT_m}{dp} = \frac{\Delta V_m}{\Delta S_m}, \quad (1)$$

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where ΔV_m and ΔS_m denote the change in volume and entropy on melting, respectively, T_m is the melting temperature, and p is pressure. Since ΔS_m must remain positive during melting, for a negative $\frac{dT_m}{dp}$ there must be negative ΔV_m . This results in a denser liquid-state along the negative melting curve compared to the solid and is the same mechanism that leads to ice floating on water.

In the liquid state, Hg is well known for its low melting point (234.3 K, -38.8°C) and for being the only metal that is liquid at ambient conditions. Mercury was also the first element discovered to exhibit superconductivity in its solid state [4]. When expanded near its liquid-vapor critical point (1750 K, 1.72 kbar), liquid Hg exhibits a metal-nonmetal transition, accompanied by dramatic changes in electronic conductivity and optical properties [5]. For this reason, extensive experimental and theoretical studies have been made to characterize the structure and properties of expanded Hg near the liquid-vapor critical point [6,7]. However, remarkably little is known about its melting behavior and structural evolution when densified at high- p conditions [3].

Diffraction measurements of liquid Hg at ambient p reveal asymmetric features in the first peak of the structure factor in reciprocal-space $S(Q)$ and real-space pair distribution functions $g(r)$ with an average coordination number of approximately 10 [8]. In contrast to strongly anomalous type-III liquid metals, Hg does not exhibit a negative melting curve on initial compression. However, the low melting point implies a melting curve minimum at negative (tensile-strained) pressure. This is supported by diffraction studies of expanded Hg near its critical point which reveal increased asymmetry in $g(r)$ and the growth of longer-range correlations attributed to the formation of nonmetallic domains [9]. The melting curve of Hg has a positive slope with increasing pressure but a flattening has been observed at around 3 to 4 GPa which may be a signature of structural or electronic reorganization in the liquid state [10]. Similar transformations have been observed in compressed Zn and In [3].

In this paper, we report *in situ* high-pressure synchrotron x-ray diffraction measurements of the melting curve of Hg and the structure of the liquid state, combined with *ab initio* molecular dynamics simulations, to determine how the local structure evolves under compression.

II. THEORY

The coherent elastic x-ray scattering of a monatomic isotropic liquid arises from a statistical distribution of interatomic separations, r , as described by the pair distribution function $g(r)$. For liquid Hg, the coherent scattering intensity per atom, $I(Q)$, can be described in terms of the pair distribution function $g_{\text{HgHg}}(r)$ by the relation

$$I(Q) = f(Q)^2 \left(1 + 4\pi\rho \int_0^\infty [g_{\text{HgHg}}(r) - 1] \frac{\sin(Qr)}{Qr} r^2 dr \right), \quad (2)$$

where $Q = 4\pi \sin \theta / \lambda$ is the elastic scattering vector for scattering angle 2θ and x-ray wavelength λ , $f(Q)$ is the single atom x-ray form factor [11], and ρ is the atomic number density. Experimentally, $I(Q)$ is obtained from the measured total scattering intensity $I_0(Q)$, corrected for background con-

tributions, according to

$$I(Q) = \frac{1}{\gamma} I_0(Q) - [f_{\text{Hg}}(Q)^2 + f_{\text{Hg}}^C(Q)], \quad (3)$$

where γ is a scaling factor to normalize $I_0(Q)$ to atomic units, and $f^C(Q)$ is the incoherent Compton scattering contribution [12].

The structure factor $S(Q)$ quantifies the atomic correlations in reciprocal space independent of the Q -dependent scattering power and is obtained by removing the form-factor envelope:

$$S_{\text{HgHg}}(Q) = \frac{I(Q)}{f_{\text{Hg}}(Q)^2} + 1. \quad (4)$$

The pair distribution function $g_{\text{HgHg}}(r)$ can be determined from the measured $S_{\text{HgHg}}(Q)$ via the inverse Fourier transform relation

$$g_{\text{HgHg}}(r) = 1 + \frac{1}{2\pi^2\rho r} \int_0^\infty Q[S_{\text{HgHg}}(Q) - 1] \sin(Qr) dQ. \quad (5)$$

The mean nearest-neighbor coordination number, $\bar{n}_{\text{Hg}}^{\text{Hg}}$, gives the average number of Hg atoms within the first coordination shell and is obtained from the area of the first peak in $g_{\text{HgHg}}(r)$ according to

$$\bar{n}_{\text{Hg}}^{\text{Hg}} = 4\pi\rho \int_0^{r_{\text{cut}}} g_{\text{HgHg}}(r) r^2 dr, \quad (6)$$

where r_{cut} is the integration cutoff for the first coordination shell, typically represented by the first minimum in $g_{\text{HgHg}}(r)$. However, if $g_{\text{HgHg}}(r)$ does not approach zero at the first minimum then the outer boundary of the coordination shell is not well defined. In this case, the resulting value of $\bar{n}_{\text{Hg}}^{\text{Hg}}$ will depend on the criterion used to define r_{cut} (e.g., by integrating to the first minimum in $g_{\text{HgHg}}(r)$ or integrating a fitted peak shape). An implicit indication of the uncertainty in $\bar{n}_{\text{Hg}}^{\text{Hg}}$ for a given method of integration is provided by the *running coordination number* function

$$\bar{n}_{\text{Hg}}^{\text{Hg}}(r) = 4\pi\rho \int_0^r g_{\text{HgHg}}(r') r'^2 dr', \quad (7)$$

which accumulates as a function of radial distance, r .

III. METHODS

A. Synchrotron x-ray diffraction (SXRD)

Simultaneous high- p - T conditions of up to 9.44(2) GPa and 659(1) K were generated using a membrane driven externally heated diamond anvil cell (DAC) equipped with Boehler-Almax type anvils with 500 μm diameter culets, surrounded by a Watlow coiled resistive heater in a vacuum vessel [13,14]. Temperature was measured using a K-type thermocouple attached to one of the diamond anvils, close to the rhenium (Re) gasket separating the anvils. Thermal gradients were minimal because the entire cell is heated from the outside. The Re gasket was preindented to approximately 25 GPa, and laser-drilled to produce a 170 μm hole, into which sodium chloride (NaCl) was compressed. A 150 μm hole was subsequently drilled through the NaCl using a mechanical microdrill. A small chip of solid Hg was broken from a bulk

sample, frozen using liquid nitrogen, and transferred into the NaCl-lined sample chamber using a cooled needle, where it melted to fill the chamber. This approach, implemented previously for liquid Ga [15], ensured that the sample was isolated from the metal gasket by the 10 μm wide annulus of NaCl, preventing Hg-Re alloying at high p - T .

Synchrotron x-ray diffraction (SXRD) measurements were made using a 56 keV monochromatic x-ray beam at beamline I15 at Diamond Light Source, UK. The incident x-ray beam was collimated using a 25 μm tungsten (W) pinhole to ensure a clean liquid signal, uncontaminated by Re or NaCl. A stepped path was followed along the Hg melting curve by increasing p and T in alternating increments up to a maximum of 9.44(2) GPa and 651(1) K, respectively. At each p - T step, the DAC was precisely aligned at the focal point of the incident x-ray beam, and short (60 s) SXRD patterns of the Hg sample were collected to constrain the melting curve by observation of liquid diffuse scattering and/or solid diffraction spots. Longer 5×240 s exposures were recorded in the liquid field just above the melting curve at approximately 1 GPa steps, up to 7.6(2) GPa and 650(1) K. After each diffraction measurement, the DAC was translated by 20–30 μm perpendicular to the x-ray beam and 60 s diffraction measurements were recorded at the edge of the NaCl ring, which served as the internal pressure calibrant. At the end of the diffraction measurements, the empty Re gasket was replaced in the DAC and diffraction measurements recorded to characterize the background contribution originating largely from Compton scattering by the diamond anvils.

At each p - T step, the unit cell volume of the B1-structured NaCl was determined from the inverse-variance weighted mean of the d spacings of a minimum of three of the following reflections: 111, 200, 220, 222, 420, 422. Pressure was then determined from this volume and the measured sample temperature with reference to the extended Mie-Grüneisen-Debye thermal equation of state of Dorogokupets and Dewaele [16] as detailed in the Supplemental Material [17].

The p -dependent structure factors, $S_{\text{HgHg}}(Q)$, and pair distribution functions, $g_{\text{HgHg}}(r)$, were obtained by normalizing the background-corrected diffraction patterns using the formalism of Eggert *et al.* [18], as implemented in the program LiquidDiffract [19], which eliminates the Q -space manifestations of the unphysical low- r contributions and provides a converged solution for the liquid atomic number density ρ .

B. *Ab initio* molecular dynamics

Ab initio molecular dynamics (AIMD) simulations of liquid Hg were performed using the Vienna *ab initio* software package (VASP) [20,21]. The electronic interactions were treated within the framework of density functional theory (DFT) using projector augmented-wave (PAW) [22,23] pseudopotentials with a [Xe] core and $5d^{10}6s^2$ valence electrons. Molecular dynamics trajectories were computed in the canonical (NVT) ensemble, with periodic boundary conditions and a Nosé thermostat [24]. Initial simulations were performed with 150, 300, and 600 Hg atoms using the Perdew-Burke-Ernzerhof (PBE) [25] exchange-correlation functional with a reference atomic number density $\rho_0 = 0.0411 \text{ \AA}^{-3}$, corresponding to a mass density of 13.69 g cm^{-3} . The systems were

heated to 3000 K for 2 ps, before equilibrating at 300 K for 15 ps with a 1 fs time step. The Brillouin zone was sampled at the Γ -point only, with a plane-wave energy cutoff of 550 eV.

The simulations containing 600 atoms were found to most accurately capture the broadening and asymmetry of the first peak in the structure factor measured at near-ambient conditions (see Fig. S3 in the Supplemental Material [17]). Hybrid Hartree-Fock/DFT (PBE0) calculations were considered to further improve agreement with the experimental data. However, these calculations were prohibitively expensive for the system sizes and timescales required to equilibrate the liquid structure. Consequently, the Armiento-Mattsson (AM05) formulation of the generalized gradient approximation (GGA) [26] was used, as it has been shown to provide results comparable to PBE0 at a fraction of the computational cost [27,28].

Further 600-atom simulations were performed using the AM05 functional at reduced atomic number densities ρ/ρ_0 up to 1.428 and temperatures up to 1500 K. The final 5 ps of each equilibrated trajectory was analyzed using the R.I.N.G.S. code to calculate the $S_{\text{HgHg}}(Q)$ and $g_{\text{HgHg}}(r)$ functions [29]. The compute time for a 5 ps calculation on the Cray XC50 Isambard-2 High Performance Computing (HPC) Service [30] was approximately nine days using eight nodes, where each node was equipped with 64 ARM-based central processing units (CPUs).

Shear viscosities (η) were calculated from the AIMD trajectories using the Green-Kubo relation formulated in terms of the integral of the stress autocorrelation function (ACF)

$$\eta = \frac{V}{k_B T} \int_0^\infty \langle \bar{P}(t + t_0) \bar{P}(t_0) \rangle dt, \quad (8)$$

where $\bar{P}$ denotes the mean of the off-diagonal components ($P_{xy}, P_{yz}, P_{zx}, \frac{1}{2}[P_{xx} - P_{yy}], \frac{1}{2}[P_{yy} - P_{zz}]$) of the traceless stress tensor, k_B is the Boltzmann constant, t is time, and the angular brackets denote an ensemble average for different time origins t_0 [31]. All ACFs converge to zero within 1 to 2 ps. The statistical error of the viscosity was estimated from the standard deviation of the values obtained for the five independent stress autocorrelation functions obtained from the individual stress tensor components.

IV. RESULTS AND DISCUSSION

A. High-pressure melting curve

The high-pressure melting curve of Hg is shown in Fig. 1. Unlike our previous study on Ga [15], in which melting curves were fitted to the center points of brackets between which the sample either melted or froze, here we find a best fit that considers the phase state observed in all of our measurements, by minimizing the *orthogonal misclassification loss*. We find that the Kechin equation [34],

$$T_m = T_0 \left(1 + \frac{(p_m - p_0)}{a} \right)^b \exp[-c(p_m - p_0)], \quad (9)$$

where T_m is the melting temperature at pressure p_m , T_0 is the melting temperature at pressure p_0 , and a , b , and c are fitted parameters and which allows for maxima, produces a much more convincing fit than the Simon-Glatzel equation [33]. In both cases, the fitted parameters are optimized using a

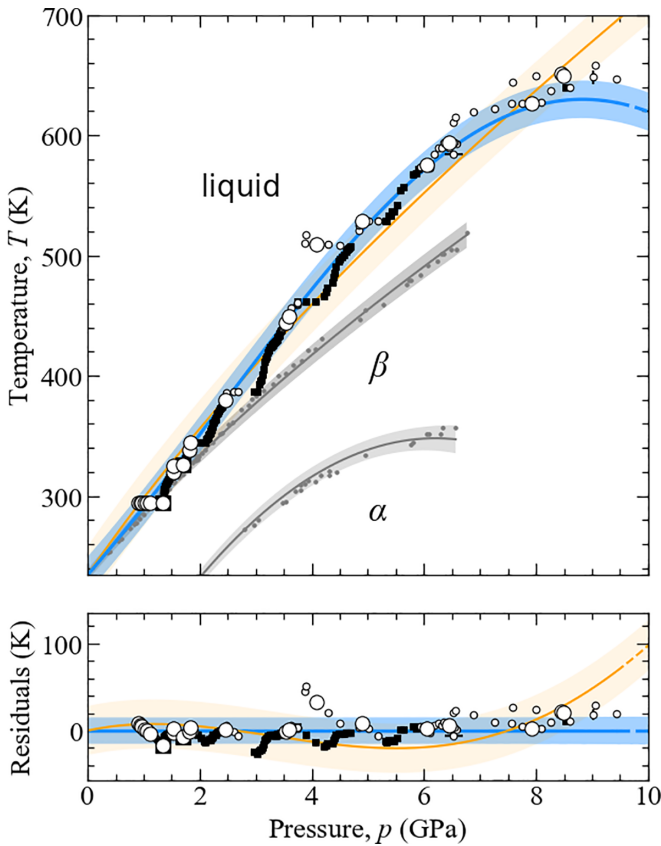


FIG. 1. Melting points of mercury (Hg) from Klement (1963) and references therein [32] are shown as gray circles; corresponding gray lines, and shaded fields represent fits to those data and their 95% prediction bands, assuming homoskedastic 1% uncertainties in both p and T . Synchrotron x-ray diffraction measurements of Hg from this study are shown as black-outlined symbols: filled squares denote solid-state data, and open circles denote liquid-state data (small symbols correspond to 60-s acquisitions; large symbols to 1200-s acquisitions for liquid structure determination). Experimental uncertainties are smaller than the symbol size in most cases. The thin orange line and shaded field correspond to the Simon-Glatzel fit [33] and its 95% prediction band, while the thick blue line and shaded field correspond to the Kechin fit [34] and its 95% prediction band. Residuals relative to the Kechin model [10] are shown in the lower panel.

loss function that seeks to identify the melting curve that best divides the dataset into its two phases, while accounting for experimental uncertainties in both p and T through orthogonal distance regression. This approach provides a robust determination of the melting boundary that prioritizes “classification correctness” rather than residual minimization alone. Optimized parameters for the fit to the Kechin equation are $a = 105.76601(2)$, $b = 315.86(1)$, and $c = 2.7563(1)$. The code used for the fitting, parameters for the Simon-Glatzel fit and covariance matrices for all the fits can be found in the Supplemental Material accompanying this paper [17].

Our new melting curve agrees with previous studies within mutual uncertainty up to ~ 2 GPa, beyond which it systematically diverges towards lower pressures at a given temperature, with the discrepancy reaching ~ 1 GPa at $T \approx 500$ K. The absence of temperature gradients in the present setup makes this

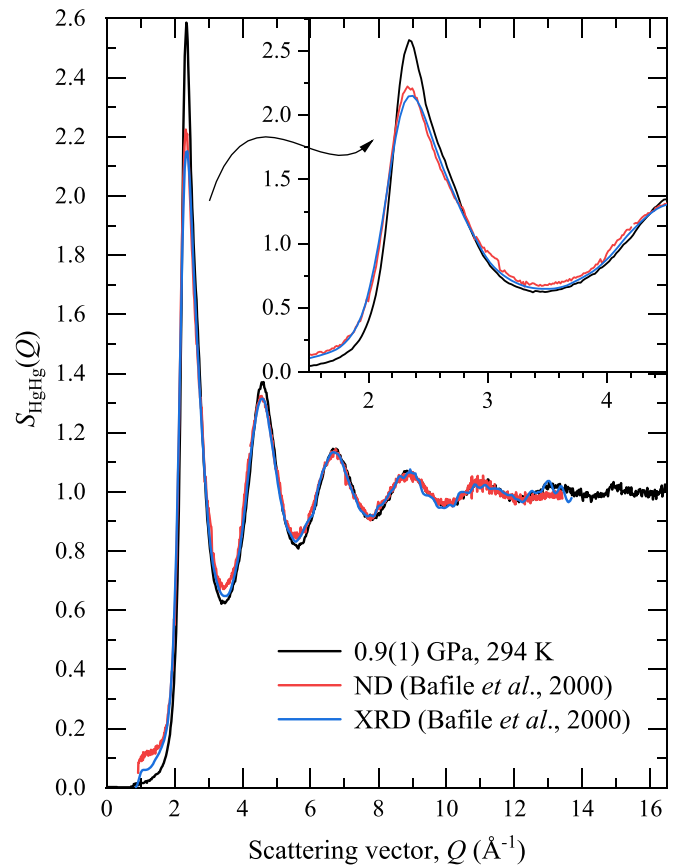


FIG. 2. Structure factor $S_{\text{HgHg}}(Q)$ of liquid Hg measured by SXRD at 0.91(1) GPa and 294 K in a membrane driven externally heated diamond anvil cell at beamline I15, Diamond Light Source (black curve). Also shown are the ambient pressure and temperature neutron (ND, red curve) and x-ray diffraction (XRD, blue curve) measurements reported by Bafle *et al.* [35].

an unlikely source of error for a mismatch of up to ~ 100 K. In contrast, the earlier measurements of Klement *et al.* [32]—and references therein—employed a piston-cylinder apparatus in which the thermocouple was offset from the sample. This configuration could lead to underestimated temperatures. Moreover, because their thermocouple was located inside the pressure vessel (unlike in our setup), its calibration may have been biased by the unquantified effects of pressure on thermoelectric electromotive force.

Regardless of these methodological differences, our results show a pronounced flattening of the melting curve beginning near 6 GPa, possibly reaching a maximum at ~ 9 GPa, followed by a negative melting slope. This behavior indicates that ΔV_m decreases over this interval and may even become negative. This trend could suggest proximity to a solid-solid-liquid triple point, but this is precluded by the topology of the subsolidus portion of the phase diagram proposed by Schulte and Holzappel [36].

B. High-pressure liquid diffraction measurements

The structure factor, $S_{\text{HgHg}}(Q)$, of liquid Hg, measured at 0.91(1) GPa and 294 K is shown in Fig. 2, together with ambient pressure neutron and x-ray diffraction measurements

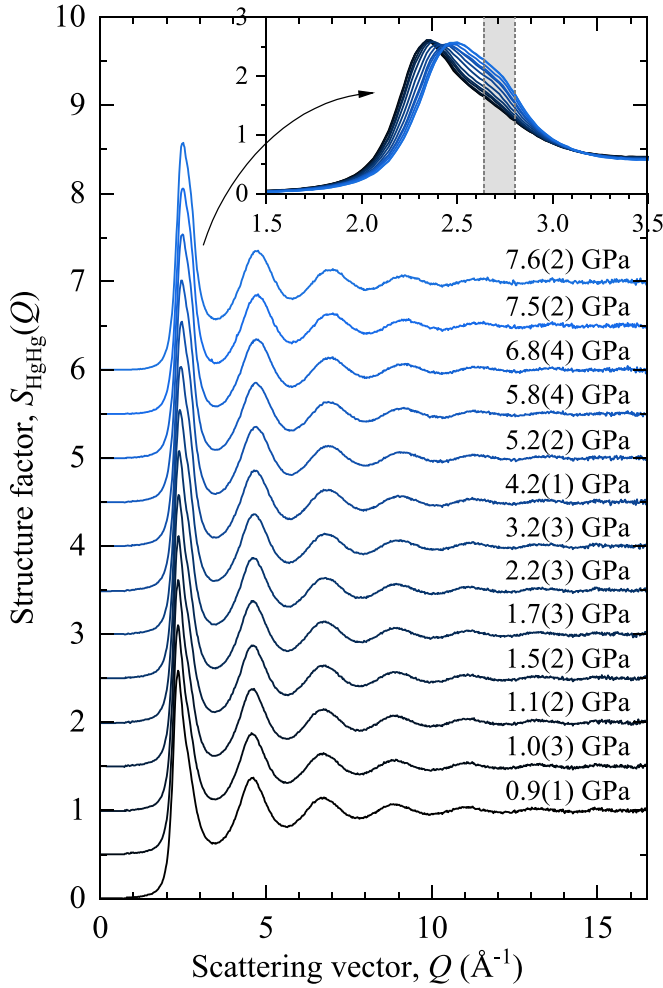


FIG. 3. Structure factor, $S_{\text{HgHg}}(Q)$, of liquid Hg as a function of pressure up to 7.6(2) GPa at 650(1) K, as measured by SXRD in a membrane driven externally heated diamond anvil cell at beamline I15, Diamond Light Source. The inset shows development of the first peak in $S(Q)$ which is sensitive to the atomic packing [3]. The shaded region indicates the estimated range of the Fermi sphere diameter, $2k_F$, over the p - T range of the experiments.

previously reported by Bafle *et al.* [35]. The present $S_{\text{HgHg}}(Q)$ function is in good overall agreement with the previous measurements, without any observable shift in the position of the first peak at $2.35(2) \text{ \AA}^{-1}$, within experimental uncertainty, notwithstanding the slight elevation in pressure. The sharper first and second peaks of the present measurement is attributable to improved instrumental resolution. In addition, the data extend to a higher momentum transfer of $16.48 \text{ \AA}^{-1}$, improving the resolution of the corresponding real-space pair distribution function $g_{\text{HgHg}}(r)$.

Figure 3 shows the high-pressure $S_{\text{HgHg}}(Q)$ structure factors of liquid Hg measured over the pressure range 0.9(1)–7.6(2) GPa at progressively increasing temperatures just above the melting curve (up to 650(1) K). With increasing pressure, the principal peak experiences a systematic shift to higher Q , from $2.35(2) \text{ \AA}^{-1}$ at 0.9(1) GPa to $2.50(2) \text{ \AA}^{-1}$ at 7.6(2) GPa, indicative of a shortening of the characteristic correlation length scale in the liquid associated with a progressive

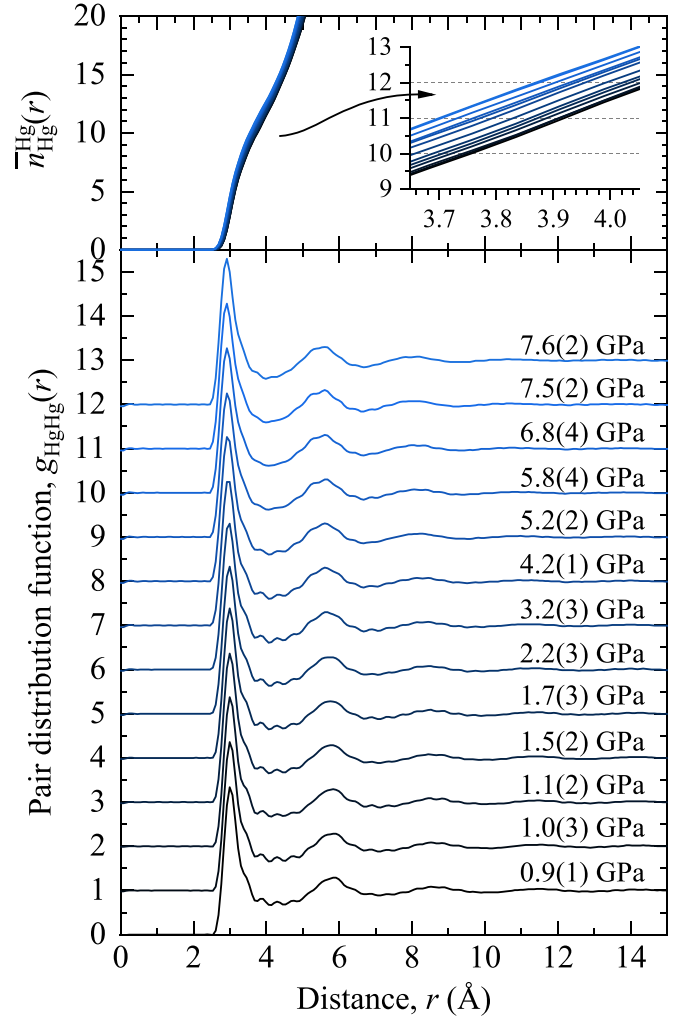


FIG. 4. Pair distribution function, $g_{\text{HgHg}}(r)$, of liquid Hg as a function of pressure up to 7.6(2) GPa at 650(1) K, as determined by a Fourier transform of the corresponding $S_{\text{HgHg}}(Q)$ data in Fig. 3. The top panel shows the running coordination number $\bar{n}_{\text{HgHg}}^{\text{H}}(r)$. The inset shows $\bar{n}_{\text{HgHg}}^{\text{H}}(r)$ in proximity to the first minimum in $g_{\text{HgHg}}(r)$.

densification of the liquid. This change is accompanied by a concomitant shift to higher Q of a broad subsidiary feature on the high- Q side of the principal peak. This subsidiary peak is a signature of topological ordering associated with low-coordinated motifs in the liquid, with a characteristic periodicity corresponding to the wavelength of Friedel oscillations [3]. The feature occurs at $Q_s = 2k_F$, corresponding to the diameter of the Fermi sphere, where k_F is the Fermi wave vector of the conduction electrons. At ambient p - T conditions $2k_F = 1.64 \text{ \AA}^{-1}$ [37] and increases with electron density, consistent with the observed shift of Q_s under compression.

Figure 4 shows the pair distribution functions $g_{\text{HgHg}}(r)$, obtained by Fourier transformation of the corresponding $S_{\text{HgHg}}(Q)$ functions shown in Fig. 3 using Eq. (5), together with the running coordination number $\bar{n}_{\text{HgHg}}^{\text{H}}(r)$ calculated using Eq. (7). At 0.9(1) GPa, $g_{\text{HgHg}}(r)$ exhibits a first peak at $r_{\text{HgHg}} = 3.00(2) \text{ \AA}$, consistent with a slight compression relative to the nearest-neighbor distances of 3.03 – $3.06 \text{ \AA}$ reported for liquid Hg under ambient (room temperature)

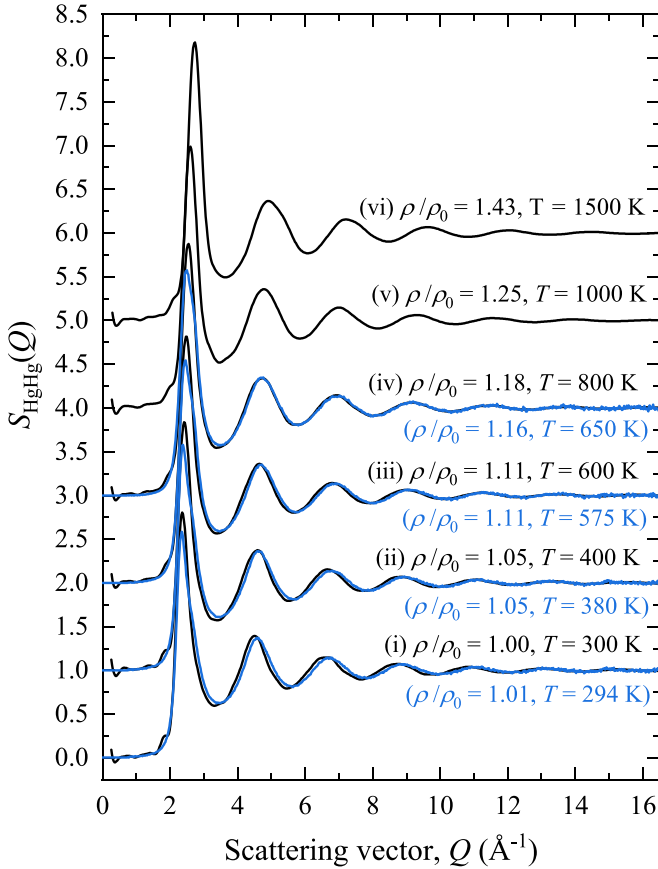


FIG. 5. Structure factors, $S_{\text{HgHg}}(Q)$, calculated from the AIMD simulations of liquid Hg at reduced densities ρ/ρ_0 and temperatures T (dark black curves). The $S_{\text{HgHg}}(Q)$ functions measured at comparable conditions in the DAC are also shown for comparison (light blue curves).

conditions [8,38]. Since $g_{\text{HgHg}}(r)$ is nonzero at the first minimum, there is no plateau in the running coordination number $\bar{n}_{\text{Hg}}^{\text{Hg}}(r)$, which precludes an unambiguous determination of the nearest-neighbor coordination. Nonetheless, integrating $g_{\text{HgHg}}(r)$ using Eq. (6) to a maximum distance $r_{\text{cut}} = 3.7 \text{ \AA}$ gives an average coordination number $\bar{n}_{\text{Hg}}^{\text{Hg}} = 9.7(4)$ at $0.9(1) \text{ GPa}$. This value is consistent with the anomalously low coordination number in the range 6–10.2 reported in early studies of liquid Hg under ambient conditions [8,38,39], indicating a departure from simple dense-packing behavior. With increasing pressure, $\bar{n}_{\text{Hg}}^{\text{Hg}}$ increases progressively reaching $11.1(4)$ at $7.6(2) \text{ GPa}$, indicating a progressive development towards more simple, hard-sphere-like packing.

C. *Ab initio* molecular dynamics

The $S_{\text{HgHg}}(Q)$ functions for liquid Hg from the AIMD simulations at conditions close to the measured melting curve are shown in Fig. 5. Given the uncertainty in simulated pressures, due to the underbinding inherent to the GGA functional, the results are presented in terms of the reduced number density ρ/ρ_0 enabling a direct comparison against the experimental data measured under comparable conditions. The corresponding real-space pair distribution functions $g_{\text{HgHg}}(r)$ are shown

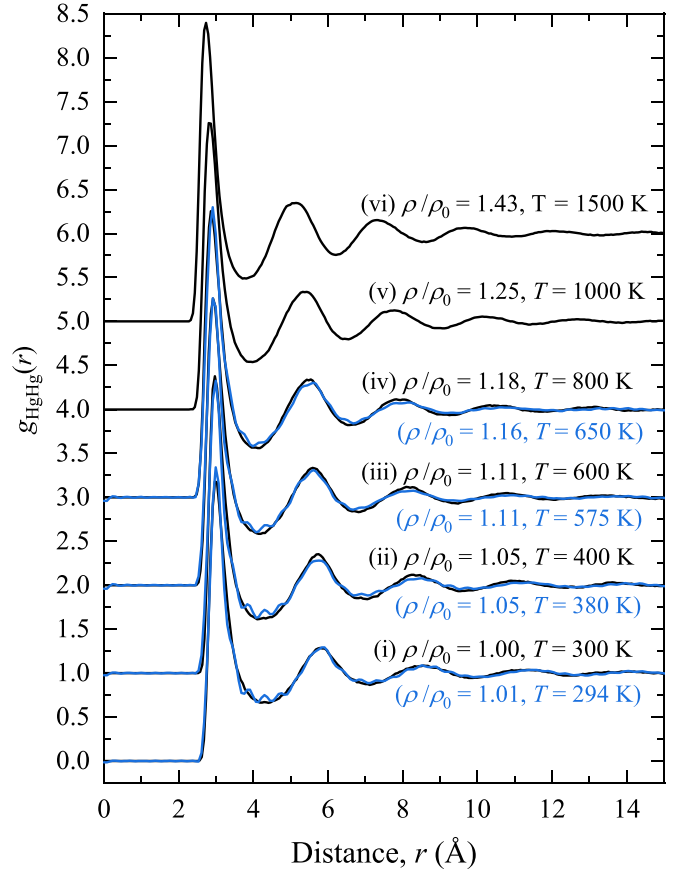


FIG. 6. Pair distribution functions, $g_{\text{HgHg}}(r)$, calculated from the AIMD simulations of liquid Hg at reduced densities ρ/ρ_0 and temperatures T (dark black curves). The $g_{\text{HgHg}}(r)$ functions measured at comparable conditions in the DAC are also shown for comparison (light blue curves).

in Fig. 6. The simulated $S_{\text{HgHg}}(Q)$ and $g_{\text{HgHg}}(r)$ reproduce the experimental peak positions and relative intensities at comparable reduced densities and temperatures, indicating that the local structure of liquid Hg is well captured by AIMD.

Figure 7(a) shows the temperature conditions investigated by SXR and AIMD as a function of reduced density, with the simulation results extending substantially beyond the experimental range of temperatures and densities. The full set of AIMD $S_{\text{HgHg}}(Q)$ functions are shown in Fig. S5 in the Supplemental Material [17].

As discussed above, because $g_{\text{HgHg}}(r)$ is nonzero at the first minimum at $\sim 4.0 \text{ \AA}$ after the first peak, there is no unambiguous mean coordination number and $\bar{n}_{\text{Hg}}^{\text{Hg}}(r)$ increases continuously (Fig. 4). Integrating to this minimum ($r_{\text{cut}} = 4.0 \text{ \AA}$) results in unphysically large coordination numbers, due to significant overlap between nearest- and next-nearest neighbor correlations. In the absence of a clear plateau in $\bar{n}_{\text{Hg}}^{\text{Hg}}(r)$, the average coordination numbers $\bar{n}_{\text{Hg}}^{\text{Hg}}$, shown in Fig. 7(b), were calculated using a constant integration limit $r_{\text{cut}} = 3.7 \text{ \AA}$ [Eq. (6)] for both experimental and simulated $g_{\text{HgHg}}(r)$ functions. This cutoff minimizes inclusion of next-nearest neighbor contributions and closely corresponds to the first minimum in $g_{\text{HgHg}}(r)$ determined by AIMD at $\rho/\rho_0 =$

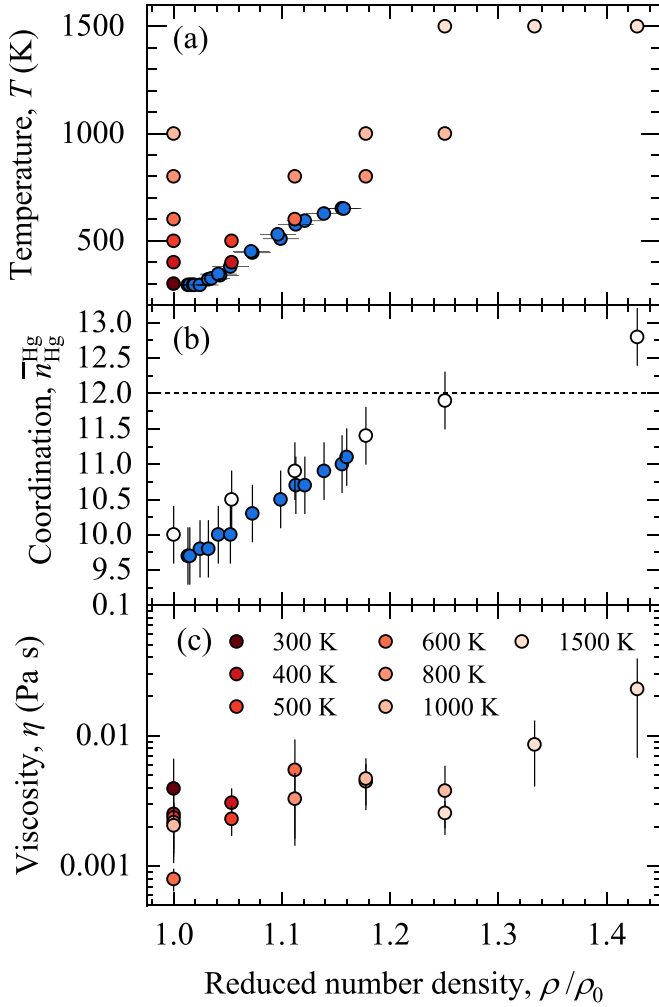


FIG. 7. (a) Temperatures of liquid Hg measurements at reduced number density ρ/ρ_0 , determined from the normalized SXR (blue circles). The temperature of the AIMD simulations are also shown (graduated red circles). (b) Average coordination number $\bar{n}_{\text{Hg}}^{\text{Hg}}$, as determined from the experimental (filled blue circles) and simulated (open circles) $g_{\text{HgHg}}(r)$ functions using Eq. (6) with integration limits $r_1 = 0$ and $r_2 = 3.7 \text{ \AA}$. The dashed line at constant coordination of 12 represents the upper coordination limit representative of a hard-sphere liquid. (c) Viscosity of liquid Hg calculated from the AIMD simulations at temperatures indicated by the legend using Eq. (8).

1.43 and $T = 1500 \text{ K}$. The error bars in Fig. 7(b) reflect the variation in coordination number obtained for small adjustments ($\pm 0.1 \text{ \AA}$) of the integration limit. The AIMD results reproduce the systematic increase in coordination number with increasing density observed in the experimental data, with $\bar{n}_{\text{Hg}}^{\text{Hg}}$ approaching the hard-sphere limit of 12 by $\rho/\rho_0 \sim 1.25$.

The simulated viscosities, shown in Fig. 7(c), remain low (in the range 10^{-3} to 10^{-2} Pa s) across the simulated conditions, comparable to the known viscosity of 1.526 mPa s for liquid Hg at ambient conditions [40]. The low viscosity, despite the high relative density of liquid Hg, reflects weak directional bonding and high atomic mobility consistent with a simple metallic liquid. Viscosity increases by an order of magnitude between $\rho/\rho_0 \sim 1$ to ~ 1.45 , consistent with an

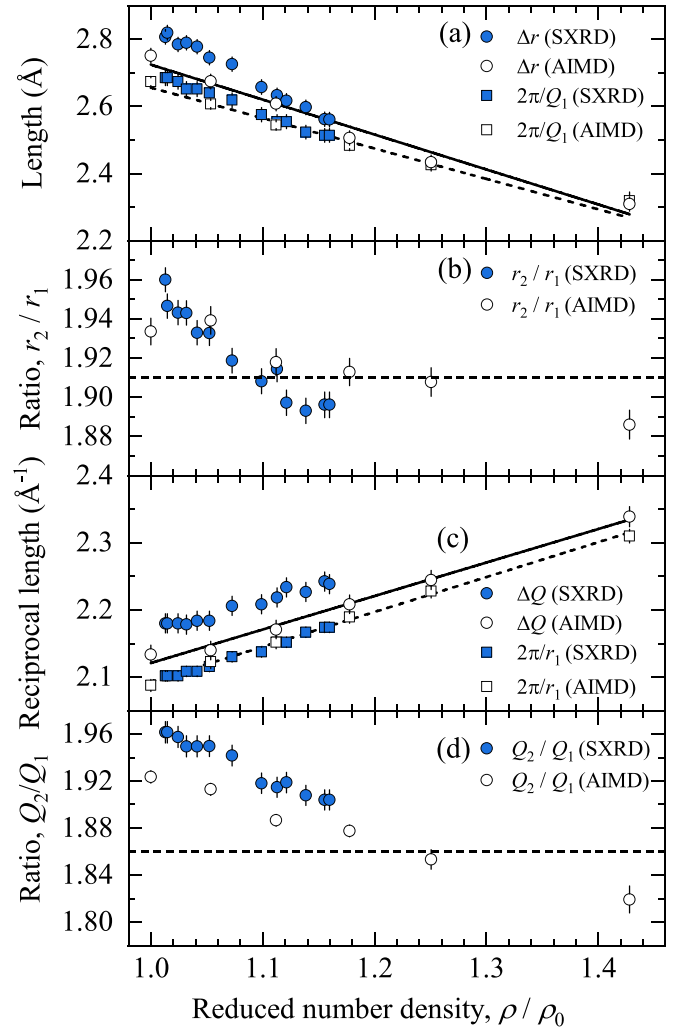


FIG. 8. (a) Medium-range real-space periodicity, Δr , at reduced number density ρ/ρ_0 determined from the $g_{\text{HgHg}}(r)$ functions measured by SXR and predicted by AIMD, compared with $2\pi/Q_1$, where Q_1 is the position of the first peak in the corresponding $S_{\text{HgHg}}(Q)$. The solid and dashed lines are linear fits to the AIMD Δr and $2\pi/Q_1$ values, respectively. (b) Ratios r_2/r_1 determined from the $g_{\text{HgHg}}(r)$ functions. The dashed line at $r_2/r_1 = 1.91$ is the ideal ratio expected for a simple hard-sphere liquid. (c) Reciprocal-space periodicity, ΔQ , determined from the $S_{\text{HgHg}}(Q)$ functions compared with $2\pi/r_1$, where r_1 is the position of the first peak in the corresponding $g_{\text{HgHg}}(r)$. (d) Ratios Q_2/Q_1 determined from the $S_{\text{HgHg}}(Q)$ functions. The dashed line at $Q_2/Q_1 = 1.86$ is the ideal ratio expected for a simple hard-sphere liquid.

increased frequency of atomic collisions at higher packing fractions. Higher temperatures generally result in lower viscosities, but the dependence is relatively weak compared to the dependence on packing density.

Figure 8 shows the relationship between reciprocal peak positions and periodicities in the experimental and simulated $S_{\text{HgHg}}(Q)$ and $g_{\text{HgHg}}(r)$ functions as a function of reduced density. The medium-range periodicity in real space, Δr , was quantified by calculating the mean pairwise atomic separation

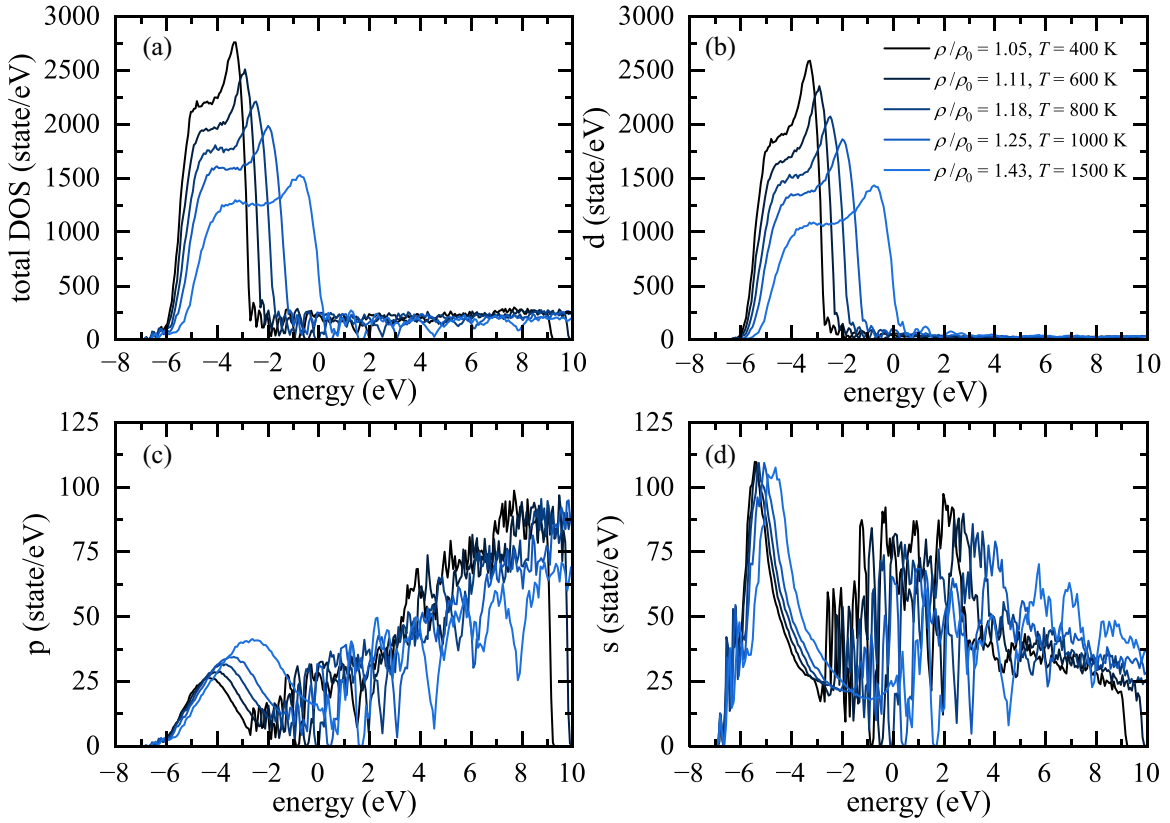


FIG. 9. (a) Total and (b) d -, (c) p -, (d) s -orbital projected electronic density of states (DOS) as calculated from the AIMD simulations of liquid Hg at reduced densities ρ/ρ_0 and temperatures T indicated in the legend.

according to

$$\Delta r = \frac{2}{n(n-1)} \sum_{i < j} \frac{r_j - r_i}{j - i}, \quad (10)$$

where r_i and r_j are the positions of the i -th or j -th peaks up to the n -th peak ($1 \leq i < j \leq n$), with each peak separation $r_j - r_i$ normalized by the number of intervening peak intervals $j - i$. As shown in Fig. 8(a), Δr converges towards the value $2\pi/Q_1$ expected for a simple hard-sphere liquid [3] with increasing density, where Q_1 is the position of the first peak in $S_{\text{HgHg}}(Q)$. The discrepancy between the experimental and AIMD Δr values at low densities is due to the slight, but observable, phase shift observed between the corresponding $S_{\text{HgHg}}(Q)$ functions at the lowest pressures, which diminishes at higher pressures (in Fig. 5).

The ratio of the first two peak positions in $g_{\text{HgHg}}(r)$ reduces from $r_2/r_1 \sim 1.95$ at ambient conditions towards the ideal hard-sphere liquid value of 1.91 [3] by $\rho/\rho_0 \sim 1.25$. An analogous relationship is observed in reciprocal-space, with the periodicity ΔQ converging towards $2\pi/r_1$ with increasing ρ/ρ_0 and the ratio Q_2/Q_1 reducing from ~ 1.94 at ambient conditions towards the ideal hard-sphere liquid value of 1.86 [3] by $\rho/\rho_0 \sim 1.25$.

A key advantage of AIMD, compared to the use of classical potentials, is the ability to directly predict the electronic structure and its development under compression. The total and orbital-projected electronic density of states (DOS) for liquid

Hg calculated from the AIMD simulations at conditions just above the measured melting curve, are shown in Fig. 9.

As shown by comparison of Figs. 9(a) and 9(b), the total DOS is dominated by contributions from the Hg 5d states. At near-ambient conditions ($\rho/\rho_0 = 1.05$, $T = 400$ K), the d -projected DOS exhibits a pronounced peak at $-3.31(2)$ eV with a broad shoulder centered at $-4.50(5)$ eV. With increasing density and temperature, this feature experiences progressive broadening, accompanied by a reduction in peak height and a systematic shift towards the Fermi energy, $E_F = 0$ eV. At the highest simulated density ($\rho/\rho_0 = 1.43$, $T = 1500$ K), the main d -DOS peak and shoulder are located at $-0.72(4)$ eV and $-3.40(5)$ eV, respectively, with a small contribution extending across E_F .

The observed change in the first peak in the structure factor and the changes in the location of the d density of states suggest there may be profound changes in the electronic properties of liquid mercury as the temperature and pressure are increased. Evans *et al.* [37,41] demonstrated that the electrical resistivity and thermopower at ambient temperature may be calculated using a modified form of the nearly free electron Ziman theory of liquid metals [42], where the weak scattering pseudopotential in simple metals is replaced by a t -matrix formulation in which the strong scattering by d states close to the Fermi energy is considered. In this case the resistivity may be written as

$$\rho_\Omega = \frac{12\pi V}{e^2 \hbar v_F} \int_0^1 \left(\frac{Q}{2k_F} \right)^3 S(Q) \left| t \left(\frac{Q}{2k_F} \right) \right|^2 \left(\frac{dQ}{2k_F} \right), \quad (11)$$

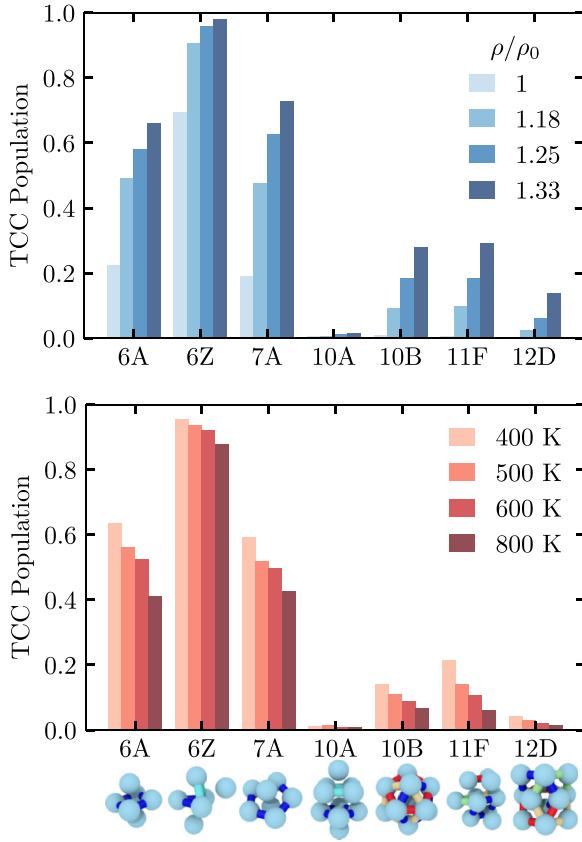


FIG. 10. Structural changes of the liquid at extreme conditions. Populations of a selection of TCC structures at $T = 1000$ K and various reduced densities (top) and reduced density $\rho/\rho_0 = 1.11$ and various temperatures (bottom). 6A and 10A clusters pick up four-membered-rings; 7A, 10B, and 12D contain five-membered rings; 11F is proto-crystalline; 6Z is a small structure in competition with 6A, and typically a precursor to five-membered ring formation. The clusters and their rings are visually depicted below the labels.

where v_F and k_F are the Fermi velocity and wave vector of the electrons, t is the scattering matrix, and $S(Q)$ is the structure factor. The t -matrix scattering is dominated by the near resonant scattering from the d states and is characterized by the η_2 phase shifts from the scattering potential. The effect of these phase shifts may be simplified to give an expression for the resistivity as [43]

$$\rho_\Omega \simeq \frac{30\pi^3 \hbar^3}{me^2 V k_F^2 E_F} S(2k_F) \frac{\Gamma^2}{\Gamma^2 + (E_0 - E_F)^2}, \quad (12)$$

where Γ and E_0 are the width and center of the d band, respectively. Equation (12) shows the resistivity depends particularly on the value of $S(Q)$ at twice the Fermi wave vector $2k_F$ and the position and width of the d -electron band. At ambient temperature and pressure $2k_F \simeq 2.64 \text{ \AA}^{-1}$ [37] that places it on the high Q side of the first peak in $S(Q)$. The inset in Fig. 3 shows $S(2k_F = 2.64 \text{ \AA}^{-1})$ increases with pressure suggesting the structural contribution to ρ_Ω also increases with pressure. However, the increase in sample density also gives rise to an increase in k_F (proportional to $\rho^{1/3}$) and E_F , with $2k_F$ estimated to be $\sim 2.8 \text{ \AA}^{-1}$ at ~ 7 GPa. Inspection of Fig. 3 suggests that $S(2k_F)$ changes only slightly between ambient

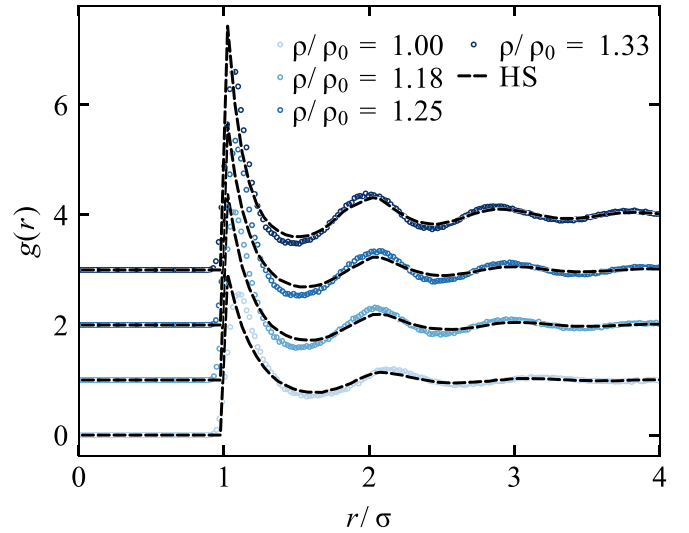


FIG. 11. Pair distribution functions from AIMD simulations compared to the hard-sphere model (HS, dashed lines) obtained via the Percus-Yevick approximation and used to infer the effective packing fractions.

and 7.6 GPa, indicating that the structural contribution to ρ_Ω is only weakly affected by pressure.

In contrast, Fig. 9 shows a substantial change in the d density of states while preserving the s and p character at the Fermi energy. The increase in the d -band broadening and the shift in the center of the d band towards the Fermi energy both give rise to an increase in ρ_Ω as the pressure increases. Indeed, the significant d contribution to the density of states at high pressure suggests a behavior similar to the first row transition metals at high pressures.

D. Topological cluster classification analysis

The three-dimensional coordinates produced by the AIMD simulations were analyzed using topological cluster classification analysis [44]. The method results in spectra of cluster populations identified by the formation of specific rings and spindle particles. The populations of the various geometrical motifs are not mutually exclusive: a particle can belong to multiple clusters at the same time. Hence, the cluster population numbers are most informative when compared across different conditions.

Figure 10 shows two example spectra for a selection of representative structures that we previously examined in a similar study of liquid Ga at extreme conditions [15]. The top series demonstrates the case of fixed temperature ($T = 1000$ K) and increasing densification. For Hg, the denser packing of the liquid leads to more motifs of increased complexity, with increases in all motif populations, similar to our previous observations for Ga. Increased packing produces a monotonic increase in the number of particles involved in the various motifs, regardless of them being fourfold symmetric (e.g., 6A) or fivefold symmetric (e.g., 7A or 10B). Liquid Hg becomes structure-rich under compression, with different motifs in competition, and similar to Ga [15]. The bottom panel of Fig. 10 presents the case of increasing temperature at reduced density $\rho/\rho_0 = 1.11$. As expected, this progressively disrupts

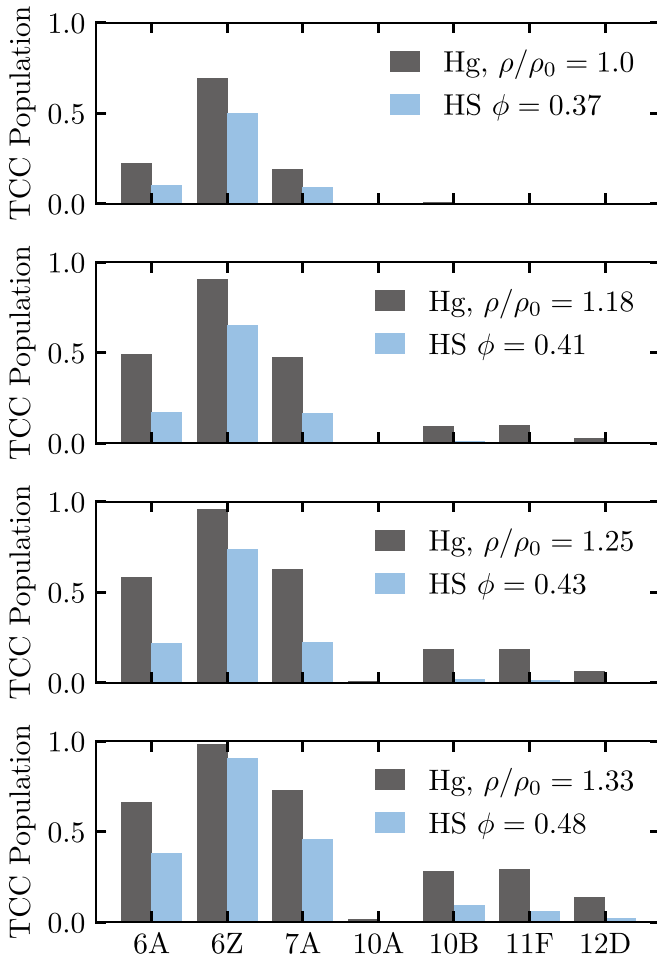


FIG. 12. Average TCC populations for Hg at $T=1000$ K under different pressures (represented by black bars) compared to populations seen in hard sphere simulations at packing fractions that most closely align with the Hg pair distribution function, according to the Percus-Yevick approximation.

the local order, as evidenced by a monotonic decrease in the fractions of particles participating in given motifs.

It is instructive to compare the obtained TCC spectra with those of the most minimal fluid model, which is the hard-sphere fluid. The hard-sphere fluid has no attractive interaction, so its phase diagram only comprises a fluid and a crystalline solid phase (FCC). Extreme conditions should be dominated by packing effects, and a comparison with hard spheres is justified. To do so, we first map the AIMD Hg simulation to monodisperse hard spheres of suitable diameters and packing fractions. We follow the analysis performed in [15] and optimize the packing fraction ϕ and effective diameter σ of model hard spheres to minimize the following objective function:

$$\mathcal{L}(\phi, \sigma) = \int_{r_0}^{r_1} [rh(r) - rh_{PY}(r; \phi)]^2 dr, \quad (13)$$

where σ is the effective diameter, ϕ the effective packing fraction, and $h(r) = g(r) - 1$ is the total correlation function extracted from the pair distribution function $g(r)$ and the PY subscript indicates the Percus-Yevick approximation used to

model the function during the fitting of σ and ϕ . This produces estimated packing fractions in the dense hard-sphere fluid regime. For example, at $T = 1000$ K, reduced densities in the range 1.00 to 1.33 map to packing fractions of 37% to 48%, which are just below the freezing limit, $\phi_f \approx 0.494$ (Fig. 11).

We can then compare the structural TCC spectra between the AIMD data and the much simpler hard-sphere model. In Fig. 12 we report this comparison at $T = 1000$ K. Some features are similar: the most frequent cluster, in the selection we have performed, is the same between the AIMD and the hard sphere data (the 6Z cluster), and all the small clusters (6A, 6Z, 7A) are represented consistently, albeit in overall smaller fractions. There is a trend toward more particles participating in more clusters as the packing fraction increases, consistent with the AIMD data at higher pressure. However, the hard-sphere configurations exhibit large clusters (e.g., the fivefold symmetric 10B, important as a locally favored structure in glass-forming systems) only at the highest packings, whereas Hg already displays them at $\rho/\rho_0 = 1.18$. This suggests that while the structural fingerprint is similar between Hg and an effective hard-sphere system, Hg presents more many-body motifs at an equivalent level of pair correlation.

V. CONCLUSION

In this work, we have used synchrotron x-ray diffraction to measure the high-pressure melting curve and liquid structure of elemental Hg to 9.44(2) GPa and 651(1) K in an externally heated diamond anvil cell. We observe a pronounced flattening, and possible maximum, in the melting curve between 6 and 9 GPa, indicating a deviation from a simple monotonic increase expected for a liquid metal. The *ab initio* molecular dynamics simulations reproduce the experimental reciprocal- and real-space correlation functions at equivalent reduced densities, demonstrating that the model provides a realistic prediction of atomistic structure of this liquid and providing confidence in its extension beyond the experimentally accessible range.

The combined experimental and simulation results reveal that, along the melting curve, liquid Hg experiences a continuous increase in local coordination and electronic delocalization, developing towards a more strongly metallic liquid state. The electronic density of states from the AIMD simulations reveals an increasing d character at the Fermi level. This is consistent with enhanced near-resonant d -electron scattering and a corresponding increase in resistivity, characteristic of the high-pressure behavior of first-row transition metals.

Despite the overall shift towards denser packing and a more metallic liquid state, topological cluster classification analysis of the AIMD trajectories reveals significant deviations from simple hard-sphere packing with larger populations of many-body clusters persisting even at the highest levels of densification. The presence of these complex motifs may provide a structural origin for the anomalous flattening of the high- p melting curve due to the emergence of metastable, low-entropy local environments, analogous to those predicted previously for liquid Ga [15].

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DATA AVAILABILITY

The data that support the findings of this article are openly available [45].

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Correction: A redundant summation term has been removed from Eq. (3).