Spectroscopic measurements of dense plasmas at billions of atmospheres provide tests to our fundamental understanding of how matter behaves at extreme conditions. Developing reliable atomic physics models at these conditions, benchmarked by experimental data, is crucial to an improved understanding of radiation transport in both stars and inertial fusion targets. However, detailed spectroscopic measurements at these conditions are rare, and traditional collisional-radiative equilibrium models, based on isolated-atom calculations and ad hoc continuum lowering models, have proved questionable at and beyond solid density. Here we report time-integrated and time-resolved x-ray spectroscopy measurements at several billion atmospheres using laser-driven implosions of Cu-doped targets. We use the imploding shell and its hot core at stagnation to probe the spectral changes of Cu-doped witness layer. These measurements indicate the necessity and viability of modeling dense plasmas with self-consistent methods like density-functional theory, which impact the accuracy of radiation transport simulations used to describe stellar evolution and the design of inertial fusion targets.
spectroscopically diagnosing classical/ideal plasmas17–20. In this regime, collisional-radiative equilibrium (CRE) models21,22 are successfully used, which combine accurate atomic data from isolated atom calculations with appropriate continuum-lowering models to describe dilute plasma effects (e.g., ionization, screening, and broadening). This approach can provide guidance, for example, on the inference of plasma density and temperature18–20. However, with increasing energy density, experimental measurements over the last decade have revealed potential inconsistencies with traditional CRE treatments.

For instance, experimental measurements1,24 on the k-edge shift of solid-density aluminum plasmas (heated by x-ray free electron lasers) favored the continuum lowering model developed by Ecker and Krohn25, while shock-compression experiments26 on the same material gave better agreement with a different continuum-lowering model by Stewart and Pyatt27. In addition, iron opacity measurements28 at pressures below 1 Mbar showed very good agreement with traditional CRE-type opacity calculations, while significant disagreements29,30 were found between measurements and theory at elevated densities and temperatures (for example, at around 10 Mbar for iron plasmas). It remains an “unsolved mystery” to this day, even though much effort has been applied to this open question from both theoretical and experimental perspectives31–33.

Today, one can accurately compute the electronic energy levels of an isolated atom by solving the many-body Schrödinger or Dirac equations, for which the calculation precision can be improved systematically by varying the sophistication of the methods that are implemented, from the simplest Hartree–Fock method to advanced multi-configuration interactions. However, when atoms are put into a non-ideal (i.e., strongly-coupled and/or degenerate) plasma environment, significant discrepancies appear between detailed spectroscopic measurements and calculations. One outstanding example is the inconsistency of hydrogen line broadening in the dilute, but cold ($n_e = 10^{10} \text{cm}^{-3}$ and $T = 10^8 \text{K}$) photospheric plasmas of white dwarfs34, in which plasma conditions inferred from the broadening of different lines in the same plasma can vary significantly, even amongst the best atomic physics models that are currently available. These variations can have significant implications for deducing the mass and age of white dwarfs by affecting the standard candle for cosmochronometry35. A similar situation occurs in warm dense plasmas under high-energy-density (HED) conditions, in which high-density effects (many-body coupling) and quantum electron degeneracy can drastically alter atomic physics relative to the isolated case. Reconciling how atomic physics changes in such non-ideal plasmas demands progress in both experiments and theory, which must account for the plasma environment self-consistently.

Over the last few years, high-resolution absorption and fluorescence spectra have been used in magnetically driven inertial fusion (cylindrical liner) experiments to study the electronic structure of warm dense matter under extreme compression36–38. These studies have shown that a self-consistent field model based on density-functional theory (DFT) could reproduce k-edge and fluorescence line shifts at independently diagnosed, imploded plasma conditions (10 eV and $n_e = 10^{21} \text{cm}^{-3}$), but collisional-radiative models with ad-hoc density effects could not reproduce the measured x-ray spectra39. A pure compression experiment without thermal or ionization effects measured density-induced shifts in the $K_\alpha$ line of cobalt at 8 Mbar, in good agreement with a self-consistent DFT model, and found significant differences among the predictions of several CRE models. It is also noted that DFT-based modeling has been successfully applied to x-ray near-edge absorption spectroscopy (XANES) for warm-dense matter38–40. These earlier XANES experiments showed absorption features in good agreement with DFT calculations38–40. Extension of these studies to gigabar pressures are very important because of their relevance to fundamental dense plasma theory, inertial fusion energy, and laboratory astrophysics.

Here, we report x-ray spectroscopy measurements at gigabar pressures using laser-driven implosions. These measurements are used to test a DFT-based multi-band kinetic model (VERITAS), which is developed in this work. The VERITAS model uses DFT-derived band (atomic level) information to compute the radiative transition rates that can be coupled to the radiation transfer equation to describe the radiative generation and transport processes in a dense plasma. With Cu (as a witness element) doped inside a 30-μm-thick plastic shell implosion, we performed time-integrated and time-resolved Cu $K_\alpha$ emission (the 2p→1s transition) and Js-2p absorption measurements during shell stagnation. Both of these inverse processes are observed on the same experiment; photo-ionization of Js electrons enables $K_\alpha$ emission, and thermal-ionization of 2p electrons enables Js-2p absorption. These observations are directly connected to the time-dependent atomic ionization balance in the assembled dense plasma. The system is further constrained by integrated measurements of the compressed areal density (pR), neutron yield and bang-time, and ion temperature, allowing the spectroscopic data to differentiate the DFT-based kinetic model from traditional treatments based on isolated-atom calculations and ad hoc continuum-lowering models.

The paper is organized as follows: first, the necessity of a reliable atomic physics model for interpreting x-ray spectroscopic measurements is demonstrated using a surrogate dense-plasma object. The experimental results are then presented with a detailed spectral comparison between measurements and simulations based on traditional atomic physics models and the DFT-based approach that is developed in this work. Finally, the implications of these results for understanding dense plasma environments are discussed.

Results

Surrogate dense-plasma object

To illustrate why a reliable atomic physics model is required a priori for interpreting dense plasma spectroscopy measurements, we construct a surrogate dense-plasma object in spherical geometry and compute synthetic x-ray spectra based on different atomic physics treatments. The surrogate plasma object consists of a 20-μm-radius core of 1% Ar-doped deuterium plasma, having a given mass density of $\rho = 10 \text{ g cm}^{-3}$ and temperature of $kT = 1000 \text{ eV}$, surrounded by four concentric homogenous shells of CH or Cu-doped CH with densities, temperatures, and thicknesses shown in Fig. 1a. The Cu-doped CH plasma serves as a “witness” layer (denoted as CHCu[2%]), which has $2%$ atomic fraction of Cu, uniformly mixed into the CH plasma.

Synthetic spectra, calculated with three different atomic physics models, are shown in Fig. 1b, c for the same CHCu[2%] density of $\rho = 20 \text{ g cm}^{-3}$, but different temperatures ($kT = 200 \text{ eV}$ and $kT = 300 \text{ eV}$, respectively). The traditional CRE simulations used an atomic database (ATBASE), implemented by the Spect3D software package, based on a kinetic description for the atomic level populations, by which levels are populated and depopulated by radiative and collisional processes, and coupled to nonlocal radiation transport. As discussed above, these CRE models need to invoke continuum-lowering models to “destroy” bound levels and account for plasma effects (pressure ionization and lowering of ionization thresholds). The remaining results in Fig. 1b, c come from VERITAS, a new DFT-based multi-band kinetic model for dense plasma spectroscopy.

The VERITAS code

The details of VERITAS can be found in Methods; here we briefly describe its essential components: (1) the electronic structure of dense Cu-doped CH plasma is determined self-consistently by DFT through quantum molecular-dynamics simulations using all-electron potentials, for a given density and temperature grid; (2) certain electronic bands, such as the Js, 2p, 3p, and continuum, are chosen to be included in the model – the oscillator strengths among these bands are calculated for the considered radiative dipole transitions; and (3) the kinetic
equation invoking the DFT-determined transition rates is used to describe the population change in these energy bands due to radiative transitions, which is coupled to the non-local radiation transport equation to ensure that the local radiation field is consistent with the band population. In contrast to a traditional CRE treatment, our DFT-based kinetic code – VERITAS–explicitly accounts for the micro-physical interactions among ions and the dense plasma environment. Energy band shifting and ionization balance are self-consistently described, without invocation of an ad hoc continuum lowering model. This model development is based on the preliminary success of treating warm-dense plasmas as quantum many-body systems\textsuperscript{39-44} with mean-field DFT.

The VERITAS predictions for the surrogate dense-plasma object prescribed by Fig. 1a are indicated by the blue solid curves in Fig. 1b, c. For the case of \( kT = 200 \text{ eV} \), Fig. 1b shows that when the hot-spot radiation streams out through the CHCu[2\%] layer, high-energy photons excite or ionize the Is core electron of Cu, leading to \( K\alpha \) emission (due to the 2p \text{\textarrow}{\text{\rightarrow}}\text{Is} transition). As the temperature of the Cu-doped layer increases to \( kT = 300 \text{ eV} \), the spectroscopic feature changes from \( K\alpha \) emission to the dominant Is-2p absorption, shown by Fig. 1c. This feature change is caused by the appreciable depletion of the Cu 2p population at this higher temperature.

\[ n_{e} = 2 \times 10^{28} \text{ cm}^{-3} \]

\( Z_{\text{Cu}} \)

\[ f_{2p} \]

\[ f_{3p} \]

\[ \mu \]

\( m \)

\( Z \)

\( \alpha \)

\( \beta \)

\( \gamma \)

The CHCu[2\%] plasma mixture has a mass density of \( \rho = 20 \text{ g cm}^{-3} \) and two different temperatures. These results are predicted from different atomic physics models. Comparisons of these predicted physical quantities demonstrate the differences between two categories of atomic physics models for warm- or hot-dense plasmas: DFT-based models vs. traditional collisional-radiative models. The quoted value of \( Z_{\text{Cu}} \) for VERITAS was calculated from the Thomas-Fermi average-atom model to provide a comparison to the other models, even though DFT calculations do not need to define \( Z_{\text{Cu}} \). Additional details of these models can be found in the Methods section.

Table 1 | Comparisons of free-electron density \((n_{e})\), average ionization \(Z'_{\text{Cu}}\), and 2p-population \((f_{2p})\) of Cu in warm- and hot-dense plasmas

| Models                  | \( kT = 200 \text{ eV} \) | \( kT = 300 \text{ eV} \) |
|-------------------------|--------------------------|--------------------------|
|                         | \( n_{e} \) \((\text{cm}^{-3})\) | \( Z'_{\text{Cu}} \) | \( f_{2p} \) | \( n_{e} \) \((\text{cm}^{-3})\) | \( Z'_{\text{Cu}} \) | \( f_{2p} \) |
| ATBASE + Stewart–Pyatt (Spect3D) | 5.1 \times 10^{28} | 13.76 | 6.00 | 5.5 \times 10^{28} | 15.78 | 5.93 |
| SCRAM + ion-sphere      | 5.1 \times 10^{28} | 14.39 | 5.84 | 5.5 \times 10^{28} | 16.37 | 5.25 |
| DFT + QMD (VERITAS)    | 5.0 \times 10^{28} | 12.88 | 5.87 | 5.3 \times 10^{28} | 14.76 | 5.27 |
| DFT + AA (Maze)        | 5.0 \times 10^{28} | 12.52 | 5.87 | 5.5 \times 10^{28} | 14.43 | 5.24 |
| FAC + AA (FAC)         | 4.2 \times 10^{28} | 12.86 | 5.87 | 4.9 \times 10^{28} | 15.19 | 5.19 |

Compared to the DFT-based VERITAS model, the two CRE models marked as “ATBASE + Stewart–Pyatt” (green dashed curve) and “ATBASE + Ecker–Kroll” (black dash-dotted curve) give quite different spectroscopic predictions for the same plasma conditions. These differences are quantitatively distinguishable: (1) the \( K\alpha \) emission peak shifts by -20 eV in the two CRE models when compared to VERITAS for the low temperature case shown in Fig. 1b; (2) the \( K\alpha \) emission peak from VERITAS is more than two-fold stronger than both CRE models, while the Ecker–Kroll model predicts a Is-2p absorption feature even at \( kT = 300 \text{ eV} \); (3) at a higher temperature of \( kT = 300 \text{ eV} \), all models predict the Is-2p absorption although the ATBASE + Ecker–Kroll model gives a wider and stronger absorption feature as indicated by Fig. 1c; and (4) at this temperature the VERITAS and Stewart–Pyatt models give a similar absorption width, but the latter shows a “double-dip” feature.

To investigate what detailed atomic physics drives these different observations, we compare in Table 1 the free-electron density, average Cu ionization \( (Z'_{\text{Cu}}) \), and Cu 2p population predicted by the following spectral models: ATBASE + Stewart–Pyatt (Spect3D - a CRE code), DFT + QMD (VERITAS), DFT + AA (Maze), FAC + AA (flexible atomic code with plasma environment inferred by an average-atom (AA) model) and one other CRE code – SCRAM. The “FAC + AA” model uses FAC-code calculations for the atomic structure of a Cu atom that is “embedded” in a CH plasma mixture in which the plasma environment is described by an average-atom (AA)-type model. It embodies a similar “spirit” to DFT with a self-consistent-field (SCF) calculation of plasma screening for an atom embedded in a plasma mixture.

The comparison indicates that both \( Z'_{\text{Cu}} \) (which governs \( K\alpha \) shifts) and the depletion of 2p (which controls the \( K\alpha \) intensity) are similar among the three DFT-based models [VERITAS, Maze, and FAC + AA]. By contrast, the traditional CRE models with similar ad-hoc continuum-lowering treatments differ from the self-consistent models and even from each other. These noticeable differences have motivated us to design and perform experiments in a similar regime, aiming to inform the development of a more-reliable HED atomic physics model for radiation generation and transport in dense plasmas.

Experimental setup and diagnostics

The experiment used a spherical, laser-driven implosion on the Omega Laser Facility. The target, shown schematically in Fig. 2a, consists of a 30-\( \mu \text{m} \)-thick polystyrene (CH) shell with a 10-\( \mu \text{m} \)-thick layer uniformly doped with 2\% Cu (atomic fraction) and a 1\% Ar-doped deuterium (D2Ar[1\%]) core fill. The 10-\( \mu \text{m} \)-thick Cu-doped layer begins ~3-
μm from the inner surface of the CH shell. The target was imploded by 60 laser beams on OMEGA with a 1-ns square pulse having a total energy of ~26 kJ. When the laser pulse irradiates the spherical capsule, laser ablation launches a strong shock wave that compresses the target. After the shock breaks out of the inner surface of the shell into the gas-filled core, the shell is accelerated inwards until it stagnates at a certain radius. At stagnation, the contained gas is compressed and heated to form a hot core, which emits x-rays that probe the stagnating shell and enable our spectroscopic measurements.

Both time-integrated and time-resolved x-ray spectrometers were used to record the emergent radiation spectrum (see Methods for further details). Figure 2b shows a typical time-resolved x-ray spectrum in the photon energy range 7800 to 8600 eV, which clearly indicates the Cu emission and absorption features of interest during the shell stagnation and core flash.

Table 2 | Comparisons of implosion performance between experiment and DRACO simulation

| Shot# 97628 | Experiment | DRACO Simulation |
|-------------|------------|------------------|
| D-D Neutron Yield | (7.3 ± 0.4)×10⁹ | 6.2×10⁹ |
| <Tᵢ>ₙ (keV) | 2.2±0.5 | 2.6 |
| <ρRₙ> (mg cm⁻³) | 67±7 | 66.5 |
| Neutron bang time (ns) | 2.04±0.05 | 2.08 |

The experimental measurements of neutron yield, neutron-averaged ion temperature, neutron-averaged areal density, and neutron bang time are compared with radiation-hydrodynamic simulations by DRACO.

Implosion performance

These high-adiabat (α = 10) and low-velocity (~250 km s⁻¹) implosions are stable to laser imprint and other perturbations, as indicated by one- and two-dimensional radiation-hydrodynamic simulations using the LILAC and DRACO codes (see below), as well as integrated experimental measurements of the implosion performance (see Table 2). Table 2 shows that the DD fusion neutron yield, neutron-averaged ion temperature <Tᵢ>ₙ, neutron-averaged shell areal density <ρRₙ> and neutron bang-time are in close agreement with LILAC and DRACO simulations. Based on these observations, we can reasonably process the radiation-hydrodynamic-simulations with atomic physics models to obtain synthetic x-ray spectra and compare them to experimental measurements.

Compared to other shocked-CH studies⁴⁵–⁵² carried out mainly along the principal Hugoniot, our experiment has extended the pressure and density conditions at which both time-integrated and time-resolved x-ray spectroscopic measurements have been conducted: gigabar (Gbar) pressures and ~15–20 × solid-density, as indicated by Fig. 2c. Inferred from DRACO simulations, the plasma temperature and density conditions of the imploding Cu-doped layer vary from kT ≈ 10⁵–50 eV and ρ ≈ 2–10 g cm⁻³ (in-flight stage) to kT = 200–500 eV and ρ = 10–25 g cm⁻³ during the stagnation.

0.6 solar mass) as it’s cooling down from hot and young state (right) to older and colder structures (left). Convective regions in the stars are shown in red. The regime probed by the experiments is shown by the green dashed circle. Inferred from DRACO simulations, the plasma temperature and density conditions of the compressed shell changes from ~50 Mbar to a maximum value approaching ~5 Gbar. When one casts these dense plasma conditions achieved on OMEGA to the density-temperature conditions of a typical white dwarf (0.6 Mₒ), during its cooling phase, Fig. 2d shows the experiment can potentially probe the equation of state and transport properties of the convective region of a white dwarf’s envelope.

![Fig. 2 | Time-resolved x-ray spectroscopy experiment of warm-/hot-dense plasmas at white dwarf's envelope conditions of Gbar pressures. a Schematic targets for implosion spectroscopy on OMEGA. b Example of streaked spectra measured in experiments. c The pressure-density region probed by various HED experiments: GEKKO⁴⁷, OMEGA⁴⁸, Nova⁴⁵, NIF by Doeppner et al.⁵¹, NIF by Kritcher et al.⁵¹, NIF by Fletcher et al.⁴⁹, as well as non-Hugoniot work by Doeppner et al.⁵⁰ on NIF. d The density-temperature conditions of a typical white dwarf of 0.6Mₒ.](https://did.gov/10.1038/s41467-022-34618-6)
Accurate knowledge about ionization balance in such conditions could directly affect the modeling of conduction and the radiative cooling of white dwarfs.

**Spectroscopic modeling**

Using the *DRACO*-simulated dynamic plasma conditions, we investigated x-ray generation and transport through the target using two *CRE* models (ATBASE and FAC) and the DFT-based kinetic code VERITAS. The predicted time-integrated spectra are compared with the experimental measurements in Fig. 3, in which the x-ray signal is plotted as a function of photon energy [all normalized to the continuum signal level at 7800 eV]. The experimental spectra (Fig. 3b) show both the spectral lines (due to less broadening), as shown in Fig. 4a. At $t = 2.05$ ns the heat wave reaches the Cu-doped layer, leading to a stronger absorption dip at lower photon energy in comparison to experiment, while VERITAS shows the same level of $1s-2p$ absorption depth.

It is noted that the experimental $1s-2p$ absorption feature is somewhat wider than in the model predictions. This slight discrepancy might come from the possibility that regions of the Cu-doped CH were driven deeper towards the hot spot by the stalk or other 3D perturbations in the experiments. Finally, when the shock and heat-wave have propagated through most of the CHCu[2%] layer, VERITAS still catches the experimental absorption level and width appropriately (Fig. 4f), while the ATBASE + Stewart–Pyatt model gives somewhat stronger absorption (green dashed curve).

**Discussion**

The spectroscopic evolution from $K_{\alpha}$ emission to $1s-2p$ absorption is directly related to the plasma conditions that are dynamically changing in the Cu-doped layer during stagnation. The density and temperature contours of the implooding shell at stagnation are respectively depicted in the upper and lower panels of Fig. 5a, as predicted by *DRACO* simulations. It shows the formation of a hot D2Ar[1%] core, with a return shock reaching the Cu-doped CH layer, and a heat wave from the hot core propagating outward by thermal conduction.

To further illustrate this process, we plot in Fig. 3b the angularly-averaged plasma density and temperature at the inner and outer...
surfaces of the CHCu[2%] layer as a function of time. One sees that the return shock reaches the inner surface of the sample layer at $t = 1.95$ ns, causing a density jump and shock heating to a temperature of $kT = 250$ eV; a heat wave follows the return shock due to strong thermal conduction from the hot core as a result of the large temperature gradient, leading to heating of the CHCu[2%] layer to $kT = 540$ eV (mid-panel of Fig. 5b); finally, the return shock approaches the outer surface of the sample layer at a later time of $t = 2.2$ ns.

Using these plasma conditions, we show the history of the Cu $2p$ band population, as predicted by VERITAS, in the lower panel of Fig. 5b.

For a fully occupied $2p$ band in Cu, there are six electrons in this band (energy level). The population of this $2p$ band starts to deplete significantly at $t = 2.0$ ns when the heat wave raises the sample layer’s temperature to over 300 eV, leading to the onset of $1s-2p$ absorption, which is observed in the time-resolved spectra (Fig. 4e). Before this time, the fully occupied $2p$ band does not allow $1s-2p$ absorption to occur, so that $K_{\alpha}$ emission is the dominant feature in the x-ray spectra measured at early times (Fig. 4d).

The plasma conditions change throughout the sample layer as the return shock and heat wave propagate through the CHCu[2%] layer.
The observed spectrum represents this competition between $K\alpha$ emission and shifted $1s$-$2p$ absorption from different radial locations. Namely, the unshocked and colder regions give pronounced $K\alpha$ emission, while the heated parts contribute dominantly to the $1s$-$2p$ absorption feature. These processes compete in generating and transporting radiation and determine what is measured by the x-ray spectrometers.

Overall, the DFT-based VERITAS model reasonably describes the dynamic change in measured x-ray spectral features. The traditional CRE models might give the proper level of both $K\alpha$ emission and $1s$-$2p$ absorption, but their predictions tend to be highly dependent on their underlying atomic structure and continuum lowering models, which can make it difficult to isolate the physical effects of interest. For these high-adiabat and relatively-low velocity implosion studies on OMEGA, it is noted that the x-ray spectroscopy data are reproducible (see Supplementary Information).

To summarize, we have performed a theoretical and experimental study of atomic physics in Cu-doped plastic at several billion atmospheres of pressure. Overall, a DFT-based approach reproduces many of the emission and absorption features that are observed in the experiment, while traditional plasma spectroscopy treatments show sensitivity to the combination of atomic physics and continuum lowering models that are implemented. This sensitivity contributes to the present open questions on the validity of ad hoc continuum lowering models (see also ref. 54). This work indicates the necessity for a self-consistent treatment of dense plasma effects on altering atomic energy levels/bands and their populations at ultrahigh pressures. The DFT-based VERITAS approach, with potential future benchmarks using other buried metal and metal-alloy layers, could provide a reliable way for simulating radiation generation and transport in dense plasmas encountered in stars and inertial fusion targets. The experimental scheme reported here, based on a laser-driven implosion, can be readily extended to a wide range of materials in single- and multiple-shell geometries, opening the way for far-reaching investigations of extreme atomic physics and DFT models at tremendous pressures.

**Methods**

**Implosion experiment on OMEGA**

The experiments were conducted by symmetric laser drive using 60 Omega laser beams. Standard implosion diagnostics were used for these experiments, including neutron yield detector\(^a\), wedge range filter for area-density measurement\(^b\), and the neutron-timing diagnostic (NTD) for ion temperature and bang time\(^c\).

**Measurement of x-ray emission spectra**

Bragg reflection crystal spectrometers recorded time-integrated and time-resolved x-ray spectra in the energy range of 7800–8600 eV. One spectrometer\(^d\) was coupled to an x-ray streak camera to achieve 80-ps time-resolution; the other was coupled to x-ray-sensitive image plate.

**Conversion to source emission.** From pinhole camera measurements of such implosions, the estimated x-ray source size is ~100-μm in diameter. With respect to the x-ray spectrometers which are 13–19 cm away from the target chamber center, the impled capsule can be represented as a point source. The measured spectra were converted to source emission $S_{\nu}^\text{ph}$ incident on each resolution element: 

$$S_{\nu}^\text{ph} = \frac{I_{\nu}}{\int_{\Omega}f_{\text{ph}}(E)dE}$$

where $I_{\nu}$ is the measured signal density (photo-stimulated luminescence (PSL) per pixel for IP and analog-to-digital units (ADU) per pixel for the streak camera), $f(E)$ the instrument sensitivity function (signal (ADU or PSL) per photon), $T(E)$ the filter transmission, and $G(E) = R(E)\frac{\text{d}E}{\text{d}E}$ the spectrometer crystal response\(^e\). $f(E)$ is constructed from calibration measurements and detector models for both the IP\(^f\) and streak camera\(^g\). The integrated reflectivity $R(E)$ is calculated from the x-ray optics software XOP\(^h\).

**Streak camera time-base.** The time-base $t(x)$ was measured on separate shots by irradiating a Au foil with a train of laser pulses of known timing. The integration time of each pixel (“dwell time”) $\Delta t = \phi_{\text{st}}$ is used to calculate the source emission rate $\phi_{\nu}$ per incident x-ray: $\frac{\phi_{\nu}}{\phi_{\text{st}}} = \frac{\Delta t}{\Delta x}$.

X-rays at the high energies of this spectrometer predominantly originate from the core; assuming the x-ray emission closely follows neutron production, the time-base is shifted to align the time of peak x-ray emission with the time of peak neutron production.

**Radiation-hydrodynamic simulations**

The radiation-hydrodynamic simulations of implosion experiments have been performed with the 1-D LILAC\(^i\) and 2-D DRACO\(^j\) codes developed at the Laboratory for Laser Energetics. State-of-the-art physics models are employed in these simulations, including 3-D ray-tracing for laser energy deposition with a cross-beam energy transfer (CBET) model\(^k\), the ISN\(^l\) nonlocal thermal transport model, and the first-principles equation-of-state (FPEOS\(^m\)) and opacity tables (FPOT\(^n\)) for constituent materials. For radiation energy transport, a multi-group diffusion model was used in DRACO with 48-group opacity tables. Cylindrical symmetry was enforced in the 2D DRACO simulations, in which $r-z$ coordinates are employed with the azimuthal symmetry axis along the $z$-axis. The quasi-1D nature of such high-adiabat implosions should lead to small 2D or 3D effects in x-ray emission calculations, justifying use of 2D (as opposed to 3D) simulations. Laser imprinting was simulated up to a maximum laser-speckle mode of $l = 150$ in DRACO, even though these simulations showed little effect of laser perturbations on such high-adiabat implosions with 1-ns square pulses at a laser intensity of $\sim 1.1 \times 10^{19}$ W cm$^{-2}$. DRACO simulation results were compared with experiments (e.g., see Table 2). The time-dependent 2-D density and temperature profiles, predicted from DRACO simulations, were used for further processing by a variety of CRE models and VERITAS, for x-ray spectral comparisons with experimental measurements.

**Collisonal radiative equilibrium (CRE) modeling**

Taking the DRACO-predicted plasma density and temperature profiles, we have applied the simulation package Spect3D\(^o\) to perform the CRE modeling of x-ray spectra from these implosions. Spect3D uses atomic databases and continuum lowering models to track energy level populations, which are coupled to nonlocal radiation transport for x-ray generation (e.g., $K\alpha$-emission of Cu), absorption, and propagation. The spectral resolving power ($E/\delta E = 1100$), temporal resolution ($\delta t = 80$ ps), and spatial resolution ($\delta x = 10$ μm) were applied to the synthetic x-ray spectra from Spect3D. In Spect3D simulations, we processed 10 equal-angle-spaced radial lineouts of DRACO-predicted density and temperature profiles along different angular directions with kinetic models incorporating detailed atomic physics and radiation transport. We then averaged the resulting spectra among radial lineouts. Given the largely 1D-like performance of such high-adiabat...
implosions (see Fig. 5a and Table 2), this quasi-2D treatment should be reasonable to avoid the time-consuming computations of 2D radiation transport with detailed atomic kinetics, for a relatively big 2D grid size of $601 \times 591$. Nevertheless, the use of 1-D radial lineouts in lieu of a full 2D or 3D analysis could be an additional cause for the small discrepancy observed in VERITAS-experiment comparisons.

**VERITAS:** DFT-based multi-band kinetic modeling

The VERITAS code, developed in this work, is based on a density-functional theory (DFT) description of energy bands in dense plasma. The kinetic modeling of multi-band populations ($n_i$) is coupled with radiation transfer, as described by the following coupled equations for the steady state condition:

$$\frac{dn_i}{dt} = -n_i \sum_{j=1}^{N} W_{ij} (I,\nu) + \sum_{j=1}^{N} n_j W_{ji} (I,\nu) = 0, \text{ for band } i$$

(1)

with $W_{ij}$ being the transition rates among the total $N$ bands considered, which may depend on the specific intensity $I(r,\nu)$ of x-rays at radius $r$ and frequency $\nu$ (e.g., for photoionization and stimulated radiative processes). Here, the line of sight is along the $z$ axis, which has an angle $\theta$ relative to the 1-D spherical radial coordinate $r$, i.e., $\mu = \cos(\theta)$.

The above rate equation describes the population change for each band at the steady state condition ($dn_i/dt = 0$), due to radiative processes. For example, the population rate of change on band $i$ (due to radiative coupling to band $j$ with $E_i>E_j$) can be defined as the sum of the depopulating term $-n_W W_{ij} (I,\nu)$ (stimulated absorption from $i$ to $j$) and the populating term $n_W W_{ji} (I,\nu)$ (spontaneous and stimulated emission from $j$ to $i$). Note that for the case of $E_i>E_j$ only the depopulating term appears in the rate equation for band $i$. Here, $n_W$ and $n_{B}$ are the maximum populations allowed for the corresponding radiative process. For instance, $n_W$ will depend on the number of “holes” (depletion) in band $i$ and the weighted population in band $j$: $n_B = \min(n_W, n_R, \eta_i, \eta_j, \eta_{E_i} \cdot \eta_B \cdot \eta_{E_j} / \eta)$ with $n_{full}$ being the fully-occupied population on band $i$ and $\eta_B$ standing for the degeneracy of band $i$. The Einstein coefficients $A$ and $B$ are related to the oscillator strength between bands $i$ and $j$, which can be calculated using DFT-determined orbitals. The frequency averaged mean radiation intensity is defined as $I_{\nu} = \int I(\nu) \times \phi_{\nu}(\nu - \nu_0) d\nu_0$, with the Voigt line profile $\phi_{\nu}(\nu - \nu_0)$ centered at the frequency $\nu_0$, corresponding to the energy gap between bands $i$ and $j$ and with line broadening models discussed later.

The emissivity $\eta(r,\nu)$ and absorption coefficient $\chi(r,\nu)$ have a dependence on the band population ($n_i$) of dense plasmas at the local grid $r$ and the radiation frequency $\nu$. The population changes on multiple energy bands are kinetically modeled by the rate equation (top equation), in which the radiative transition coefficients between different energy bands are calculated by using the DFT-determined orbitals, in contrast to the use of atomic databases of isolated atom plus continuum lowering in traditional CRE models. The DFT-based rate equation is then coupled with the radiation transfer equation (bottom equation) to simulate x-ray photoionization, emission, and band-band absorption processes throughout the density-temperature grid given by radiation-hydrodynamic codes. The radiation field at any spatial grid is determined by self-consistently solving the coupled rate and radiation transfer equations until a steady-state solution of the populations is achieved, similar to the procedure employed in Spect3D.

Since the DFT description of energy bands in dense plasmas is self-consistent with the plasma environment, the band energy shift is naturally included for a given plasma condition. So, there is no need to invoke a continuum lowering model in VERITAS.

In principle, many energy bands can be included in VERITAS, without prescribing which are bound and which belong to the continuum, even though such a designation can be determined from density-of-state (DOS) calculations. Specifically, we have included the measurement-relevant energy bands $[1s, 2p, 3p, \text{and continuum of copper (Cu)}]$ for modeling the implosion spectroscopy experiments. The main radiative processes considered among Cu’s energy bands are: 1s $\leftrightarrow$ continuum (photoionization/radiative-recombination), 2p $\leftrightarrow$ 2p (band-band absorption/K$_s$-emission). 1s $\leftrightarrow$ 3p (band-band absorption/K$_p$-emission). 2p $\leftrightarrow$ continuum (photoionization/radiative-recombination), and 3p $\leftrightarrow$ continuum (photoionization/radiative-recombination). Even though we are focusing on the 1s $\leftrightarrow$ 2p transition spectra, the inclusion of the bounded 3p-band of Cu is to ensure that all relevant population and depletion channels of the 1s-band are properly accounted for in the kinetic simulations. The exclusion of 2s and 3s bands from VERITAS modeling of the current experiments is based on the fact that their transitions to the 1s band are dipole-forbidden and their coupling to 2p and 3p are outside the spectral range of interest. At the plasma conditions encountered here, the $n=4$ bands of Cu have already merged into the continuum. For the conditions studied here ($20 - 500$ eV and $2 - 20 \times$ solid-density), the rates for electron collisional processes are so high that local thermodynamic equilibrium is well maintained. Thus, one can take the thermal-DFT predicted band populations as a starting point in VERITAS to simulate the aforementioned radiative processes only, while the fast electron collisional processes are assumed to balance each other so that they can be omitted from current VERITAS simulations.

To enable the VERITAS simulations of these x-ray spectroscopy experiments, we have first built a DFT-based table storing the relevant frequency and oscillator strength of transitions among Cu’s energy bands, for a density and temperature grid of $\mathrm{CHCu}[2\%]$ spanning the mass density and temperature ranges of $\rho=2-50$ g cm$^{-3}$ and $kT=10-500$ eV. For each density and temperature condition, we have performed quantum molecular-dynamics (QMD) simulations to sample a variety of ionic configurations of dense CHCu[2%] plasma, based on the thermal-DFT formalism in either the Kohn-Sham orbital-based format or the orbital-free scheme. These DFT-based QMD calculations have been performed by using ABINIT$^2$ and our in-house OFMD code (DRAGON), with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional$^2$. For temperatures below $50$ eV the QMD simulations were done using the orbital-based Kohn-Sham DFT implemented in ABINIT, while for high temperatures ($kT > 50$ eV) we turned to orbital-free DFT to perform our QMD simulations. Taking snapshots from QMD calculations, we performed the oscillator strength calculations for radiative transitions by using the Kubo-Greenwood package - KEGC@QUANTUM-ESPRESSO$^7$, with the all-electron projector-augmented-wave (PAW) potential$^8$. These choices of DFT packages, exchange-correlation functional, and potentials follow standard practice in the warm-dense matter physics community. The band-energy deficiency from DFT calculations has been compensated with constant shifts derived from comparison with experimental energy levels of Cu at ambient condition. The band-energy “deficiency” from DFT refers to the small ($\sim 2\%$) difference between the DFT-calculated $1s-2p$ energy gap of Cu and the experimentally measured $\text{Ka}$ energy at ambient conditions. This small band-gap difference has been known as an intrinsic fact of DFT that uses approximated exchange-correlation functionals (e.g., PBE used here) which suffer from self-interaction error. These DFT calculations invoked $100-200$ atoms of C, H, and Cu according to their atomic fractions in a supercell with periodic boundary conditions, which were converged with respect to number of bands, K-points, and energy cut-off.

With such a pre-calculated DFT table accessible to VERITAS, the radiative transition rates can be computed at any spatial grid for plasma conditions of $\text{CHCu}[2\%]$ given by rad-hydro simulations. It is
noted that the kinetic modeling was done only for the sample CHCu[2%] layer, while radiation transport in D2Ar and pure CH plasmas were calculated by using the emissivity and opacity tables from PrOpacEOS76, same as what were used in CRE modeling. In principle, the band broadening of Cu can be determined from direct DFT-based QMD calculations. However, due to the limited number of Cu atoms involved in such demanding calculations, the resulting band-width (broadening) is currently not reliable due to the lack of sufficient sampling for charge-state distribution (CSD). Instead, we have adopted in VERITAS the temperature- and density-dependent broadening information coming from both SCRAM48 and FAC72 calculations for Stark (with an enhancement factor of ~5) and CSD broadening effects, as well as Doppler shift due to fluid motion, in a Voigt line profile. Both the SCRAM and FAC codes consider traditional plasma broadening mechanisms, including electron thermal-collision broadening73. Stark broadening due to ion micro fields74, and broadening from the charge-state distribution69. While all of these broadening mechanisms can explain the line-shape observations in low-density and high-temperature classical plasmas, they appear unable to account for the enhanced broadening seen in the dense plasmas created and reported here. We speculate that the current treatment of micro-field induced Stark broadening might have missed some of the density effects from coupled ions in such dense plasmas, hence the ad-hoc 5x increase in broadening applied to the VERITAS results. We hope the experimental observations of enhanced broadening reported here shall motivate future investigations on how density effects change line broadening in warm-dense plasmas. Finally, since VERITAS is based on the DFT description of dense plasmas, we expect its low-density limit to be around or slightly below ambient solid density, below which DFT calculations are no longer practically feasible and traditional atomic physics models should work better.

Data availability
The experimental data, Spec3D simulation data, VERITAS simulation data that support the findings of this study are available from the corresponding authors upon request.

Code availability
The VERITAS code that support the findings of this study are available from the corresponding authors upon request.

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Author contributions
S.X.H. and P.M.N. conceived the project and wrote the initial manuscript. D.T.B., D.A.C., and P.M.N. performed the experimental measurements. S.X.H. developed the DFT-based VERITAS code and performed the DFT calculations, with help from I.E.G., V.V.K., S.B.H., D.I.M., N.R.S., and S.Z. The Spect3D calculations were performed by M.G., I.E.G., and T.W.; S.B.H. provided the SCRAM and Muze calculations. M.G. performed the FAC calculations. All authors discussed the results and revised the manuscript.

Competing interests
The authors declare no competing interests.

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