Thermophysical properties of warm dense hydrogen

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We study the thermophysical properties of warm dense hydrogen using quantum molecular dynamics simulations. New results are presented for the pair distribution functions, the equation of state, the Hugoniot curve, and the reflectivity. We compare with available experimental data and predictions of the chemical picture. Especially, we discuss the nonmetal-to-metal transition which occurs at about 40 GPa in the dense fluid.

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I. INTRODUCTION

Hydrogen is an essential element for models of stellar and planetary interiors. The isotopes deuterium and tritium are considered as target materials (D-T gas) in inertial confinement fusion experiments. Therefore, numerous efforts have been made both experimentally and theoretically to understand the behavior of hydrogen, deuterium, and tritium in a wide range of densities and temperatures. In particular, progress in shock-wave experimental technique has allowed the systematic probing of the megabar pressure range, so that a sound database has been assembled within the last decade. Single or multiple shock-wave experiments have been performed for hydrogen (or deuterium) by using, e.g., high explosives, gas guns, pulsed power, or high-power lasers. The combination of high pressures and temperatures of several eV defines warm dense matter, a strongly correlated state relevant for planetary interiors which is characterized by partial ionization where the bound states exhibit a highly transient nature.

Furthermore, the enormous progress in computer capacity has allowed the development and application of ab initio simulation techniques for warm dense matter such as Path Integral Monte Carlo (PIMC) or Quantum Molecular Dynamics (QMD) simulations which treat quantum effects and correlations systematically. These techniques give already highly predictive results for a variety of problems and systems; see Ref. 12 for QMD simulations.

The equation of state (EOS) and derived quantities such as the Hugoniot curve, the sound velocity, or the Grüneisen parameter are important material properties in this context. Furthermore, optical properties as, e.g., the reflectivity are closely related to the dielectric function which also determines the dc electrical conductivity in the static limit. All these quantities are used to characterize the unique behavior of warm dense hydrogen, especially for high pressures at, or exceeding, one megabar, where a transition from a nonconducting, molecular fluid to a mono-atomic fluid with metallic-like conductivity occurs. Describing the disordered fluid in terms of solid state parameters, the fundamental band gap between the valence and conduction band decreases with the pressure and, subsequently, the electrical conductivity shows an exponential increase as is typical for thermally activated transport in semiconductors. For pressures above 1.4 Mbar, conductivities of about 2000 Ω cm is characteristic for simple metallic fluids such as Cs, have been observed experimentally around 3000 K, and band gap closure has been claimed to be responsible for this nonmetal-to-metal transition.

On the other hand, concepts of plasma physics have been applied to warm dense matter states. For instance, the chemical picture gives a rather simple description by identifying stable bound states out of elementary particles as new composite particles. Hydrogen at normal conditions in this context is a molecular fluid. Free electrons are generated at high pressure by dissociation of molecules, H$_2$ = 2 H, and a subsequent ionization of atoms, H = e + p. This model yields already the strong increase of the conductivity with the pressure (pressure ionization). In addition, bound states contribute to conduction via hopping processes. The conceptual problem of all chemical models is the clear definition of bound states, the derivation of effective potentials between all species, and the calculation of cross sections for the respective scattering processes in a strongly correlated medium.

QMD simulations are a powerful tool to describe warm dense matter. The combination of classical molecular dynamics for the ions and density functional theory (DFT) for the electrons allows one to consider correlation and quantum effects. Alternatively, wave packet simulations have been developed in which the electrons are represented on a semi-quantal level by wave packets (WPMD).

In this paper, we apply QMD simulations and calculate
a broad spectrum of thermophysical properties of warm dense hydrogen. We determine EOS data for a wide region of densities and temperatures and compare with chemical models. We calculate the principal Hugoniot curve for liquid targets. The Kubo-Greenwood formula serves as a starting point for the evaluation of the dynamic conductivity $\sigma(\omega)$ from which the dielectric function $\varepsilon(\omega)$ and the reflectivity can be extracted. In addition, the electronic structure calculation within DFT yields the charge density distribution in the simulation box at every time step, and the molecular dynamics run gives valuable structural information via the ion-ion pair correlation function. This is important for the identification and characterization of phase transitions such as solid-liquid or liquid-plasma as well as for the nonmetal-to-metal transition.

II. QMD SIMULATIONS

Within QMD simulations we perform molecular dynamics simulations with a quantum mechanical treatment of the electrons by using density functional theory (DFT). This is based upon the theorems of Hohenberg and Kohn and gives the electron density that minimizes the ground state energy of the system. It has been proven that this density is a unique functional of the effective potential $V_{\text{eff}}$.

From this formalism Kohn and Sham derived a computational scheme which solves the problem for a fictitious system of non-interacting particles that leads to the same electron density. This scheme consists basically of solving the Kohn-Sham equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(r)\right] \varphi_k(r) = \epsilon_k \varphi_k(r), \quad (1)$$

$$V_{\text{eff}}[\varrho(r)] = \int \frac{g(r')\varrho(r')}{|r-r'|} dr' - \sum_{k=1}^{N} \frac{Z_k^2 \alpha^2}{|r-k|} + V_{\text{XC}}[\varrho(r)].$$

Our ab initio quantum molecular dynamics simulations were performed within Mermin’s finite temperature density functional theory (FT-DFT)\cite{323534}, which is implemented in the plane wave density functional code VASP (Vienna Ab Initio Simulation Package)\cite{323534}. We used the projector augmented wave potentials\cite{2334} and did a generalized gradient approximation (GGA) using the parameterization of PBE\cite{32}. Extensive test calculations, as performed already by Desjarlais\cite{22}, have shown that the EOS data are dependent on the plane wave cutoff. A convergence of better than 1% is secured for $E_{\text{cut}} = 1200$ eV which was used in all actual calculations. The electronic structure calculations were performed for a given array of ion positions which are subsequently varied by the forces obtained within the DFT calculations via the Hellmann-Feynman theorem for each molecular dynamics step. This schema is repeated until the EOS measures are converged and a thermodynamic equilibrium is reached.

The simulations were done for 64 atoms in a supercell with periodic boundary conditions. The temperature of the ions was controled by a Nosé thermostat\cite{25} and the temperature of the electrons was fixed by Fermi weighting the occupation of bands\cite{26}. The Brillouin zone was sampled by evaluating the results at Baldereschi’s mean value point\cite{27} which showed best agreement with a sampling of the Brillouin zone using a higher number of k-points. The density of the system was fixed by the size of the simulated supercell. To achieve a small statistical error due to fluctuations the system was simulated 1000-1500 steps further after reaching the thermodynamic equilibrium. The EOS data and pair correlation functions were then obtained by averaging over all particles and simulation steps in equilibrium. Similar calculations were performed recently for the thermophysical properties of warm dense helium\cite{28} in order to verify the nonmetal-to-metal transition at high pressures.

The zero-point vibrational energy of the H$_2$ molecules is not included in DFT calculations. In previous calculations, the energy $\frac{1}{2} \hbar \omega_{\text{vib}}$ per molecule is simply added which is very important, especially at low temperatures and for the calculation of an exact initial internal energy for the reference state of the Hugoniot curve, which is 0.0855 g/cm$^3$ at 20 K. To account for this quantum effect more sensitively for arbitrary temperatures, the fraction of molecules has to be derived, e.g., for all states along the Hugoniot curve. This can be done via the coordination number

$$K(r) = \frac{N - 1}{V} \int_0^r 4\pi r^2 g(r')dr',$$  

which is a weighted integral over the pair correlation function $g(r)$ of the ions. $N$ denotes the number of ions and $V$ the volume of the supercell in the simulation. The doubled value of $K$ at the maximum of the molecular peak in $g(r)$, which is found around $r = 0.748$ Å, is then equal to the fraction of ions bound to a molecule and twice the amount of molecules in the supercell. An example is shown in Fig. 1 where the increasing dissociation with higher density can be seen. In Fig. 2 we show the thermal dissociation; the molecular peak dissappears with increasing temperature at constant density. Note that the peak is thermally broadened.

The dissociation degree is calculated for a number of isotherms and then approximated by a Fermi function which has two adjustable parameters. These parameters can be represented by temperature-dependent functions so that the dissociation degree and, subsequently, the contribution of molecules to the zero-point internal energy are determined for arbitrary temperatures. The results show that molecules can be neglected above 10,000 K.

We compare the resulting dissociation degree with that derived by Vorberger et al\cite{30} in Fig. 3. They counted all pairs of atoms in a range of 1.8 a$_B$ as atoms. In a second step they reduced the number of molecules by counting only those pairs that are stable for longer than ten vibra-
III. RESULTS FOR THE EOS AND HUGONIOT CURVES

We show the thermal EOS of warm dense hydrogen in Fig. 4. The isotherms of the pressure show a systematic behavior in terms of the density and temperature. We find no indication of a plasma phase transition (PPT) which would result in an instability of the EOS isotherms that would need to be treated by a Maxwell construction. The absence of a PPT is in contrast to results of chemical models which use, e.g., Fluid Variational Theory (FVT) or liquid state perturbation theory. Chemical models are based on a free energy minimization schema for a mixture of hydrogen atoms, molecules, and a plasma in chemical equilibrium. Correlations are taken into account based on effective two-particle potentials. The description of the free charged particles (plasma) is done beyond the Debye-Hückel approximation by using efficient Padé formulas which are valid for a wide region of densities and temperatures.

In Fig. 4 our QMD results are compared with the chemical models FVT and SCvH-i. The EOS derived by Saumon et al. shows also a PPT (SCvH-ppt data set). The modified SCvH-i data set shown here avoids the PPT by using an interpolation through the instability region. Therefore, both data sets can be used to study the influence of a PPT on interior models of giant planets such as Jupiter. Consistent chemical models yield the correct low-temperature and low-density limit and agree with our QMD results there. A good agreement is also found in the high-density limit where a nearly temperature independent behavior characteristic of a degenerate plasma is found. At medium densities the pressure isotherms of FVT and SCvH-i lie well below the QMD data; the deviations amount up to 25%.

We have encountered a region with \((\partial P/\partial T)_V < 0\), which was previously reported by Vorberger et al. It can be related to the rapid dissociation transition at low temperatures.

Following Lenosky et al. and Beule et al. we fit smooth functions for the pressure \(P\) and the internal energy \(U\) as an expansion in terms of density \(\rho\) and tem-
perature to the given results of the QMD simulations. The pressure is split into an ideal and an interaction contribution:

\[ P = P_{\text{id}} + P_{\text{int}} = \frac{p k_B T}{m_H} + P_{\text{int}}(\rho, T). \]  

(3)

The QMD data for the pressure \( P \) given in kbar can be interpolated by the following expansion for the interaction contribution:

\[ P_{\text{int}}(\rho, T) = (A_1(T) + A_2(T)\rho)A_0(T), \]  

(4)

\[ A_j(T) = a_{i0} \exp \left( -\frac{(T-a_{i1})}{a_{i2}} \right)^2 + a_{i3} + a_{i4}T. \]  

(5)

The coefficients \( a_{i,k} \) are summarized in Tab. I.

The QMD data for the specific internal energy \( u = U/m \) given in kJ/g can be interpolated by a similar expansion:

\[ u = \sum_{j=0}^{4} B_j(T)\rho^j, \]  

(6)

\[ B_j(T) = b_{j0} \exp \left( -\frac{(T-b_{j1})}{b_{j2}} \right)^2 + b_{j3} + b_{j4}T. \]  

(7)

The expansion coefficients \( b_{j,k} \) are given in Tab. II.

The expansions (1) and (6) reproduce the \textit{ab initio} QMD data within 5% accuracy in a density range from 0.5 g/cm\(^3\) to 5 g/cm\(^3\) between 500 K and 20000 K and can easily be applied in planetary models or hydrodynamic simulations for warm dense matter. The expansions fulfill thermodynamic consistency expressed by the relation

\[ P - T \left( \frac{\partial P}{\partial T} \right)_V = - \left( \frac{\partial U}{\partial V} \right)_T. \]  

(8)

FIG. 4: Thermal EOS for warm dense hydrogen (pressure isotherms): QMD data are compared with the chemical models FVT \(^{44}\) and SCvH-i \(^{45}\), within 15% accuracy which is mainly due to the deviations from the QMD data itself.

A crucial measure for theoretical EOS data is the principal Hugoniot curve which is plotted in Fig. 5. It describes all possible final states \( (\rho, P, u) \) of shock wave experiments according to the Hugoniot equation

\[ u - u_0 = \frac{1}{2} \frac{(P + P_0)(\frac{1}{\rho_0} - \frac{1}{\rho})}{\rho_0} \]  

(9)

starting at the same initial conditions \( (\rho_0, P_0, u_0) \). For the hydrogen principal Hugoniot curve, the initial density is \( \rho_0 = 0.0855 \text{ g/cm}^3 \) and the initial internal energy \( u_0 = -314 \text{ kJ/g} \) at a temperature of 20 K. The initial pressure \( P_0 \) can be neglected because of the high pressure of the final state.

Shock wave experiments have been performed for deuterium using gas guns \(^{48}\) magnetically launched flyer plates at Sandia’s Z machine \(^{49}\) or high explosives (HE) \(^{50}\). These experiments indicate a maximum compression of 4.25 at about 50 GPa.

Another series of laser-driven experiments \(^{48}\) shows systematic deviations from the experiments quoted above. Especially, a maximum compression of 6 has been reported at about 1 Mbar. According to the unanimous evaluation of the shock-wave experimental data for molecular liquid \(^{51}\), we compare our QMD data in Fig. 5 only with the data sets mentioned above.

The systematic increase of the cutoff energy \( E_{\text{cut}} \) in QMD simulations from 500 eV \(^{52}\) to 1200 eV \(^{53}\) has lead to fully converged results in agreement with the experimental points. The consideration of the zero-point vibrations of the H\(_2\) molecules along the entire Hugoniot curve yields a very good agreement of QMD data with the gas gun experiments \(^{54}\), especially for low pressures. The calculated Hugoniot curve has a maximum compression of 4.5 which is slightly higher than the HE and Z experiments indicate (about 4.25). This is an agreement of about 5% accuracy which can be translated into an accuracy of about 1% in the measured shock and particle

| TABLE I: Coefficients \( a_{i,k} \) in the expansion for the pressure \( P_{\text{int}} \) according to Eqs. (1) and (6). |
| --- | --- | --- | --- | --- | --- |
| \( i \) | \( a_{00} \) | \( a_{11} \) | \( a_{22} \) | \( a_{33} \) | \( a_{44} \) |
| 0 | 0.2234 | 2919.84 | 3546.67 | 1.94023 | 1.11316 \times 10^{-6} |
| 1 | 14.7586 | 2117.98 | 4559.17 | -17.9538 | 4.88041 \times 10^{-4} |
| 2 | -33.8469 | 2693.63 | 4159.13 | 70.582 | -2.8848 \times 10^{-4} |

| TABLE II: Coefficients \( b_{j,k} \) in the expansion for the specific internal energy \( u \) according to Eqs. (1) and (6). |
| --- | --- | --- | --- | --- |
| \( j \) | \( b_{00} \) | \( b_{11} \) | \( b_{22} \) | \( b_{33} \) |
| 0 | -33.8377 | 2154.38 | 3696.89 | -300.446 | 1.77956 \times 10^{-2} |
| 1 | 55.8794 | 3174.39 | 2571.21 | 56.222 | -3.56234 \times 10^{-3} |
| 2 | -30.0376 | 3174.02 | 2794.39 | 87.3659 | 2.0819 \times 10^{-3} |
| 3 | 5.57328 | 3215.51 | 2377.23 | -13.1622 | -3.84004 \times 10^{-4} |
| 4 | -0.3236 | 3245.48 | 2991.45 | 0.682152 | 2.19862 \times 10^{-5} |
velocity, which is in the range of the systematic errors in the experiments. The compression decreases with higher pressures and temperatures and reaches the correct high-temperature limit as given by the PIMC simulations\textsuperscript{[53,54]. The QMD curve lies slightly below the experimental data for compression rates between 3 and 4 which could be due to the known band gap problem of DFT in GGA. The FVT curve\textsuperscript{[55,56]} is shown as a representative of chemical models which, in general, show a higher compressibility well beyond 4.5.

Also shown is the linear mixing result of Ross\textsuperscript{[57]. This curve shows a sixfold compression and is not in agreement with the shown experiments. The curve of Kerley\textsuperscript{[58]} has a maximum compression of 4.25, like the experiments indicate, but the pressure is there slightly higher than the results of the QMD simulations.

FIG. 5: Principal Hugoniot curve for hydrogen. The results of this work (solid line) are compared with previous QMD results of Lenosky \textit{et al.}\textsuperscript{[59]} (dashed) and Desjarlais\textsuperscript{[60]} (stars), PIMC simulations\textsuperscript{[61]} (dotted), the linear mixing model of Ross\textsuperscript{[62]} (dot-dash-dashed), the model of Kerley\textsuperscript{[63]} (dot-dotted-dashed) and the chemical model FVT\textsuperscript{[64]} (dot-dashed). Experiments: Gas gun\textsuperscript{[65]} (diamonds), Sandia Z machine\textsuperscript{[66]} (grey squares; grey line: running average through the $u_e-u_p$ data), high explosives\textsuperscript{[67]} (black circles).

**IV. DYNAMIC CONDUCTIVITY, REFLECTIVITY AND DC CONDUCTIVITY**

The dynamic conductivity $\sigma(\omega)$ is derived from the Kubo-Greenwood formula:\textsuperscript{[55,56]}

$$\sigma(\omega) = \frac{2\pi e^2 \hbar^2}{3m^2\omega^2} \sum_k W(k) \frac{\sum_i \sum_j \sum_{\alpha=1}^N [F(\epsilon_{i,k}) - F(\epsilon_{j,k})]}{\sqrt{\sum_{\alpha=1}^N |\Psi_{j,k}^\alpha|^2}}$$

$$\times \left[ |\Psi_{j,k}^\alpha|^2 |\Psi_{i,k}^\alpha|^2 \right] \delta(\epsilon_j - \epsilon_i - \hbar\omega),$$

(10)

where $e$ is the electron charge and $m$ its mass. The summations over $i$ and $j$ run over $N$ discrete bands considered in the electronic structure calculation for the cubic supercell volume $\Omega$. The three spatial directions are averaged by the $\alpha$ sum. $F(\epsilon_{i,k})$ describes the occupation of the $i$th band corresponding to the energy $\epsilon_{i,k}$ and the wavefunction $\Psi_{i,k}$ at $k$. The $\delta$-function has to be broadened because a discrete energy spectrum results from the finite simulation volume\textsuperscript{[21]. Integration over the Brillouin zone is performed by sampling special $k$ points\textsuperscript{[57]}, where $W(k)$ is the respective weighting factor. We used Baldereschi’s mean value point\textsuperscript{[38]} to reach a convergence of better than 10% accuracy.

Optical properties can be derived from the frequency-dependent conductivity Eq. (10). The standard method is to obtain the imaginary part via the Kramers-Kronig relation

$$\sigma_2(\omega) = \frac{2}{\pi} \frac{P \int \sigma_1(\nu)\omega}{(\nu^2 - \omega^2)} d\nu,$$

(11)

$P$ is the principal value of the integral. The dielectric function can be calculated directly with the conductivity:

$$\epsilon_1(\omega) = 1 - \frac{1}{\epsilon_0\omega^2} \sigma_2(\omega),$$

(12)

$$\epsilon_2(\omega) = \frac{1}{\epsilon_0\omega^2} \sigma_1(\omega).$$

(13)

The square of the index of refraction contains the real part $n$ and the imaginary part $k$ is equal to the dielectric function which leads to the following relations:

$$n(\omega) = \frac{1}{2} \sqrt{\epsilon(\omega) + |\epsilon_1(\omega)|},$$

(14)

$$k(\omega) = \frac{1}{2} \sqrt{\epsilon(\omega) - |\epsilon_1(\omega)|}.$$

(15)

The index of refraction is then used to calculate optical properties such as the reflectivity $r$:

$$r(\omega) = \frac{1}{1 + n(\omega)^2} + \frac{k(\omega)^2}{1 + n(\omega)^2} + k(\omega)^2.$$  

(16)

We compare our \textit{ab initio} results with reflectivities measured along the Hugoniot curve\textsuperscript{[28]} in Fig. 5; the agreement is excellent. The change of the hydrogen reflectivity with the pressure can be interpreted as a gradual transition from a molecular insulating fluid through an atomic fluid above 20 GPa where the atoms have strongly fluctuating bonds with next neighbors\textsuperscript{[20]} to a dense, almost fully ionized plasma with a reflectivity of about 50-60 % at high pressures above 40 GPa. The chemical model\textsuperscript{[29]} shows also this qualitative behavior but the abrupt increase of the reflectivity occurs at a higher density. This shows the difficulties of the chemical models in finding the correct shifts of the dissociation and ionization energies as function of density and temperature and, thus, the location of the nonmetal-to-metal transition. However, the limits of a molecular fluid at low pressures and of a fully ionized plasma at high pressures are incorporated in a reasonable way.
can be used easily in, e.g., hydrodynamic simulations for warm dense hydrogen and in astrophysical applications.

The results show a smooth transition from a molecular liquid to an atomic fluid of metal-like state. There were no signs of a PPT which is predicted by other models.

With these EOS results we have calculated the principal Hugoniot curve which is in agreement with dynamic experiments and has the correct high-temperature limit as given by PIMC simulations.

We obtained optical properties using the Kubo-Greenwood formula. The reflectivity along the Hugoniot curve is in excellent agreement with experiments. The results show the occurrence of a nonmetal-to-metal transition at about 40 GPa.

V. CONCLUSION

We have performed ab initio QMD simulations to study thermophysical properties of hydrogen under extreme conditions. As a result we obtained highly converged EOS data which are relevant for modeling giant planets and for the understanding of the fundamental behavior of hydrogen at high pressure. The deviations between our QMD data and chemical models amount up to 25%. We have constructed smooth fit functions for the QMD data for the pressure and the internal energy which

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