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A MASSIVE CORE IN JUPITER PREDICTED FROM FIRST-PRINCIPLES SIMULATIONS

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ABSTRACT

Hydrogen-helium mixtures at conditions of Jupiter's interior are studied with first-principles computer simulations. The resulting equation of state (EOS) implies that Jupiter possesses a central core of 14–18 Earth masses of heavier elements, a result that supports core accretion as the standard model for the formation of hydrogen-rich giant planets. Our nominal model has about 4 Earth masses of planetary ices in the H-He-rich mantle, a result that is, within a modeling uncertainty of 6 Earth masses, consistent with abundances measured by the 1995 *Galileo* entry probe mission, suggesting that the composition found by the probe may be representative of the entire planet. Interior models derived from this first-principles EOS do not give a match to Jupiter's gravity moment J_4 unless one invokes interior differential rotation, implying that Jovian interior dynamics has an observable effect on the high-order gravity field.

Subject headings: dense matter — equation of state — planets and satellites: individual (Jupiter)

Online material: color figures, machine-readable table

1. INTRODUCTION

The discovery of over 200 extrasolar planets resembling the giant planet Jupiter in mass[5] and composition (e.g., Burrows et al. 2007) has raised fundamental questions about the origin and inner structure of these bodies. Establishing the existence of a dense core in Jupiter is vital for understanding the key processes of planetary formation. An observed correlation between the metallicity of the parent star and the likelihood of giant planets orbiting it (Fischer & Valenti 2005) may indicate that an initial core aggregated from solid planetesimals triggers the gravitational collapse of nebular gases to form giant planets (Mizuno 1980), or alternatively, increased metallicity enhances the direct collapse of giant planets from the nebula (Mayer et al. 2007). Current planetary models (Saumon et al. 1995; Saumon & Guillot 2004) predict only a very small core between 0 and 7 Earth masses ($M_\oplus$) for Jupiter, lending support to core-accretion theories with comparatively small cores (Pollack et al. 1996) or to late-stage core erosion scenarios (Guillot et al. 2004), or suggesting that Jovian planets are able to form directly from gases without a triggering core (Boss 2007). Using first-principles simulations for hydrogen-helium mixtures at high pressure, we show here that Jupiter possesses a significant central core of $16 \pm 2\ M_\oplus$ of heavier elements, a result that supports core accretion as the standard model for formation of hydrogen-rich giant planets. In our model, Jupiter's mantle, defined as the H-He-rich outer layers, shows no enrichment of heavier elements, indicating that compositional measurements from the 1995 *Galileo* entry probe mission may be representative of most of the planet. The derived interior models also provide the first evidence that Jupiter's interior does not rotate as a solid body because no match to Jupiter's gravity moment J_4 is obtained unless one invokes interior differential rotation, implying that Jovian interior dynamics have an observable effect on the measured gravity field.

While laboratory techniques cannot yet probe deep into Jupiter's interior (reaching pressures $P \sim 100$–1000 GPa and temperatures $T \sim 10000$ K), advances in first-principles computer simulation techniques have made it possible to characterize the equation of state (EOS) of hydrogen-helium mixtures for the entire planet. The determination of the EOS, in combination with the modeling reported here, enables us to more precisely specify Jupiter's mantle metallicity and core mass.

2. SIMULATION METHODS

All density functional molecular dynamics (DFT-MD) simulations were performed with either the CPMD code[6] using local Troullier-Martins norm-conserving pseudopotentials or with the VASP code (Kresse & Hafner 1993) using the projector augmented-wave method (Blöchl 1994). The nuclei were propagated with ground-state Born-Oppenheimer MD because simulations with thermally excited electrons did not yield any significant correction to the EOS in Jupiter's interior. Exchange-correlation effects were described by the generalized gradient approximation (Perdew et al. 1996). The orbitals were expanded in a plane-wave basis with a 35–50 Ha energy cutoff. The simulations were run for 2 ps with time steps between 0.2 and 0.8 fs. We performed well over a hundred separate DFT-MD simulations on a nonuniform grid in density and temperature ranging from $\rho = 220$ to 6006 kg m^{-3} and from 500 to 20000 K. At lower densities, we used classical Monte Carlo simulations with fitted potentials (Ross et al. 1983), which are in very good agreement with the Saumon–Chabrier–Van Horn (SC) EOS (Saumon et al. 1995; Chabrier et al. 2006).

All simulations were performed with 110 hydrogen and 9 helium atoms in periodic boundary conditions. The initial simulations were performed with Γ point sampling of the Brillouin zone only. Further simulations with uniform grids of up to $4 \times 4 \times 4$ k-points exhibited a correction to the pressure in the metallic regime. This correction slowly increases with density, eventually reaching -1.6% at conditions of Jupiter's core. Finite size effects were further analyzed by Vorberger et al. (2007b). The isentropes were derived from a thermodynamically consistent fit to the free energy (Militzer 2008).

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[5] J. Schneider, the Extrasolar Planets Encyclopedia, http://exoplanet.eu.

[6] 1990–2006, copyright IBM Corp., MPI für Festkörperforschung Stuttgart 1997–2001.

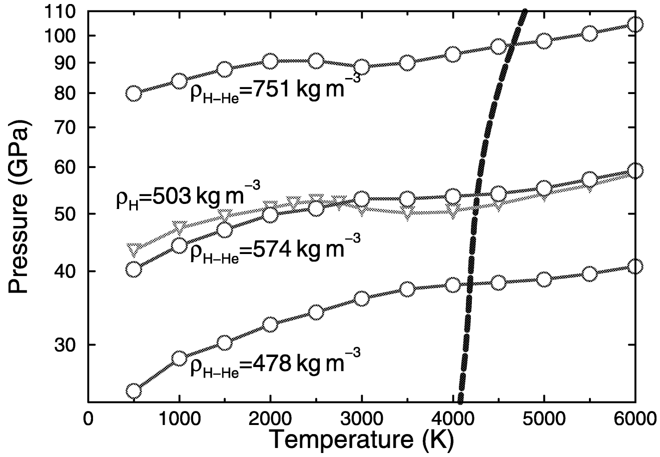

FIG. 1.—Isochores derived from DFT-MD simulations of H-He mixtures (*circles*; $Y = 0.2466$) and pure hydrogen (*triangles*). Results for mixtures predict a positive Grüneisen parameter, $(\partial P/\partial T)|_V > 0$, along Jupiter's isentrope (*dashed line*) predicting the planet to be isentropic and fully convective. [*See the electronic edition of the Journal for a color version of this figure.*]

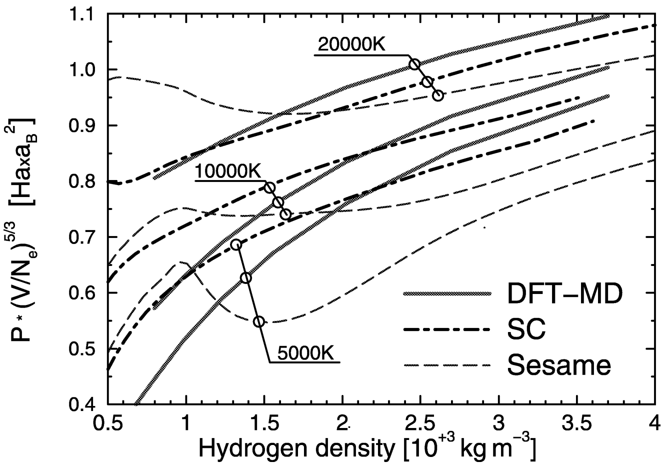

FIG. 2.—Comparison of the DFT-MD EOS with the SC and Sesame models. Three isotherms for pure hydrogen are shown in the metallic regime at high pressure. P is scaled by the volume per electron to the power 5/3 to remove most of the density dependence. [*See the electronic edition of the Journal for a color version of this figure.*]

DFT-MD predicts a continuous transition from the molecular to a dissociated regime in fluid hydrogen as function of pressure (Vorberger et al. 2007a, 2007b), which is consistent with quantum Monte Carlo simulations (Delaney et al. 2006). The dissociation transition in dense hydrogen is driven by the increasing overlap of molecular orbitals. At sufficiently high compression, Pauli exclusion effects trigger a delocalization of the electronic charge (Militzer 2005), the band gap closes (Vorberger et al. 2007a, 2007b), the conductivity increases, the protons are no longer paired, and eventually the system assumes a metallic state (Johnson & Ashcroft 2000). As the temperature of the fluid increases, this transition occurs at lower pressures due to stronger collisions. When helium is added to dense hydrogen, it localizes the electronic charge because of its stronger binding. It dilutes the hydrogen subsystem by reducing overlap of molecular orbitals, increasing the stability of hydrogen molecules compared to pure hydrogen at the same P and T (Vorberger et al. 2007b).

While the DFT-MD EOS has a positive compressibility for all P and T, such that $(\partial P/\partial \rho)_T > 0$ (where ρ is the mass density), the method predicts a negative Grüneisen parameter, equivalent to $(\partial P/\partial T)_\rho < 0$, for the dissociation region of pure hydrogen (Vorberger et al. 2007a, 2007b). A negative Grüneisen parameter would introduce a convection barrier into Jupiter's mantle. However, Figure 1 demonstrates that in a H-He mixture, the region where $(\partial P/\partial T)_\rho$ is negative occurs at higher pressures and significantly lower temperatures than are present in Jupiter's interior. Consequently, Jupiter's mantle is predicted to be fully convective and isentropic.

3. INTERIOR MODELS

Were Jupiter of exactly solar composition and all its magnesium-silicates and iron together with the abundant hydrides CH_4, NH_3, and H_2O concentrated in a dense core, considering recent reductions in the solar C and O abundances, its core mass would only comprise about 3 $M_\oplus$ (Grevesse et al. 2007). The core mass thought to trigger nebular collapse is several times larger (Mizuno 1980). Detection of a central core with a resolution of a few $M_\oplus$, only 1% of Jupiter's total mass of 318 $M_\oplus$, places stringent demands on the accuracy of the hydrogen-helium EOS. We show in this Letter that an EOS based on DFT-MD differs from the previous SC EOS by considerably more than 1%.

Figure 2 compares the DFT-MD results for pure H with the SC EOS. The SC model relies on analytical techniques that describe hydrogen as an ensemble of stable molecules, atoms, free electrons, and protons. Approximations are made to characterize their interactions. Conversely, with DFT-MD one simulates a fully interacting quantum system of over a hundred electrons and nuclei. The isotherms shown in Figure 2 specify the EOS in the inner regions of Jupiter where hydrogen is metallic. Due to the lack of experimental data at this density, predictions from chemical models including the Sesame database (Lyon & Johnson 1992) vary substantially. The DFT-MD method obtains higher densities than the SC EOS for much of the pressure range characteristic of the interior of Jupiter. This has great influence on the predicted core mass. Moreover, DFT-MD predicts a continuous molecular-to-metallic transition while the original SC EOS model predicts this transition to be of first order, which introduced the possibility of having different chemical compositions in the inner and outer layers of Jupiter. Guillot et al. (1997) showed that having flexibility to redistribute materials allows one to make a coreless model for Jupiter while typical models with constant chemical composition in the mantle predict a core of about 7 $M_\oplus$ when the SC EOS is used. Conversely, our DFT-MD EOS predicts Jupiter's mantle to be isentropic, fully convective, and of constant chemical composition. As we show below, the mantle metallicity is so low that compositional gradients would be unlikely to change this conclusion.

Jupiter isentropes from different models are compared in Figure 3. The chemical composition corresponding to each isentrope was determined by adding 1 mass percent of CH_4 and NH_3, and 0.5% of H_2O (collectively called "planetary ices"; Nellis et al. 1997), using ideal mixing, to the mixture of H and He considered here. The adequacy of the ideal-mixing approximation was verified by simulations with "guest atoms" of C, N, or O. The H-He DFT-MD EOS was derived for a single He mass fraction $Y = 0.2466$, to be contrasted with the Jovian atmospheric He mass fraction (as a fraction of H and He only) measured by the *Galileo* entry probe, $Y = 0.238 \pm 0.005$ (von Zahn et al. 1998). The DFT-MD isentrope was then perturbed to the probe He abundance by using ideal mixing with a pure He density at the same

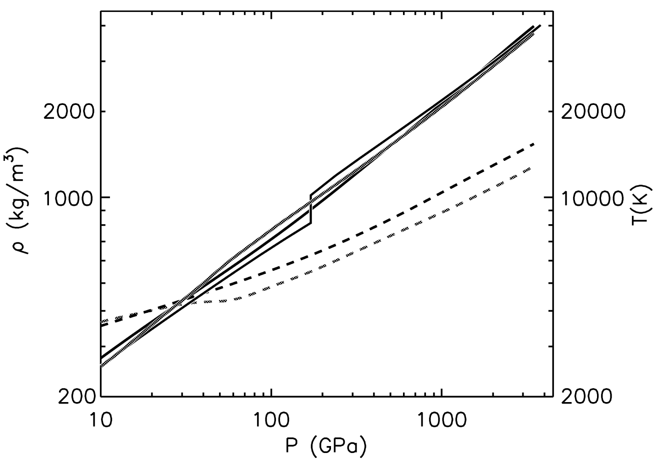

Fig. 3.—Comparison of the resulting Jupiter models. Solid curves show mass density (*left-hand ordinate*) and dashed curves show temperature T (*right-hand ordinate*), as a function of pressure P. In contrast to Fig. 2, the DFT-MD (*red line*) and the SC models have differing chemical compositions and temperatures at each pressure. The outermost layers at $P < 100$ GPa make about 90% of the contribution to the gravity moment J_4. The black curves show two models based on the smoothed and discontinuous versions of the SC EOS. [*See the electronic edition of the Journal for a color version of this figure.*]

T and P, synthesized from separate DFT-MD simulations for pure helium (Militzer 2008). As can be seen in Figure 3, DFT-MD implies lower temperatures in the deep Jovian interior in isentropic models, further contributing to generally increased density with respect to SC models. The high density requires us to adopt $Y = 0.238$ throughout the mantle. Figure 3 compares the original discontinuous as well as the smoothed SC EOS version that we use in Figure 2 and discuss below.

The DFT-MD EOS yields a significant revision of the interior structure of Jupiter. The resulting model predicts a large central core of 16 $M_\oplus$ and a low metallicity for the mantle while models based on the SC EOS imply a small core and a much higher metallicity in the mantle, comprising some tens of $M_\oplus$ of elements heavier than H and He (Saumon & Guillot 2004; Guillot et al. 1997). DFT-MD based models predict that the planetary ices were primarily incorporated into a massive solid core and depleted gaseous nebula. Conversely, models based on the SC EOS imply that planetary ices were largely accumulated along with the nebular hydrogen and helium when Jupiter formed. Figure 3 shows that the Jupiter model based on the DFT-MD EOS is about 5% denser than the model based on the smoothed SC EOS over the pressure range 30 GPa $< P <$ 300 GPa, which spans about 30% of the mass of Jupiter, while it is a few percent less dense at deeper layers. The *Galileo* probe found abundances of CH_4, NH_3, and H_2O (at the deepest level) corresponding to at most about 6 $M_\oplus$ of planetary ices if extrapolated to the entire mantle (Niemann et al. 1998; Wong et al. 2004). Our nominal model achieves a fit with 4 $M_\oplus$ of planetary ices in the mantle and is consistent with such an extrapolation of the Galileo measurements but modeling uncertainty of the ice fraction is comparable to its value itself.

If Jupiter formed in a region of the solar nebula where temperatures were too low for H_2O to be in the gas phase, it would follow that a primordial core would include most of the H_2O in solid form, and that accreted nebular gas would accordingly be depleted in H_2O. This is consistent with the last model in Table 1. We estimate that the non-H-He component of Jupiter's mantle comprises 4 ± 2 $M_\oplus$, and Jupiter's dense core comprises 16 ± 2 $M_\oplus$. The error bars include systematic and statistical uncertainties in the DFT-MD EOS. The dense core is modeled as rock and H_2O in solar proportions, but could for example include 4 $M_\oplus$ of sedimented He for an initial $Y = 0.25$. Simulation parameters were chosen in order to reach an accuracy of 1% within the DFT method. A uniform 1% alteration of the pressure changes the core mass by 1 $M_\oplus$. An earlier Jupiter model based on a completely different set of DFT-MD EOS results for pure hydrogen (Vorberger et al. 2007b) yielded a core mass that differed by 2 $M_\oplus$. A 1% increase in the temperature at the 1 bar level increases the mantle ice content by 1 $M_\oplus$. We use these differences to estimate the uncertainties of our predictions.

An acceptable model of Jupiter's interior must match the observed constraints of the planet's mass, equatorial radius at a standard pressure of 1 bar, and the observed multipole moments J_2, J_4, and J_6 of the gravity field normalized to the equatorial radius. Jupiter's multipole moments are primarily a response to the planet's rotation, and the higher order moments can be strongly affected by nonuniform rotation. Traditional models of Jupiter's interior structure and external gravity have assumed solid-body rotation equal to the rotation rate of the magnetic field (rotation period is 9:55:29.7 hours, stable over decades; Seidelmann 1992). Our model calculations find the axially symmetric mass density through a self-consistent field (SCF), calculated to fourth order in the rotational distortion (Hubbard et al. 1975; Hubbard 1982). We incorporate differential rotation on cylinders to the same order as the SCF. Table 1 shows that models with solid-body rotation and the DFT-MD EOS predict a $|J_4|$ that is seven standard deviations larger than the observed $|J_4|$. The error bar of J_4 has decreased by about a factor three[7] with respect to earlier determinations (Campbell & Synnott 1985). As predicted by theory (Anderson et al. 1974), reduced $|J_4|$ is associated with a more rapid decrease of density with radius in the pressure range 1–100 GPa. However, we have no physical justification for making ad hoc modifications to the $P(\rho)$ relation in this pressure range. Since we have a fully convective mantle in our model, we cannot match J_4 by distributing helium unevenly in an upper and lower mantle layer, which is one major difference compared to earlier models (e.g., Saumon & Guillot

[7] R. A. Jacobson (2003), JUP230 orbit solution, http://ssd.jpl.nasa.gov/?gravity_fields_op.

TABLE 1
Constraints on Jupiter's Interior Structure and Parameters of Models Based on DFT-MD EOS

Model	Equatorial Radius (km)	Gravity Moments $J_2 \times 10^6$	$J_4 \times 10^6$	$J_6 \times 10^6$	Core Mass ($M_\oplus$)	Mantle Ice ($M_\oplus$)	T at CMB[a] (K)	P at CMB[a] (GPa)
Observed	71492	14696.43 ± 0.21	-587.14 ± 1.68	34.25 ± 5.22	…	…	…	…
Solid-body rotation	71492	14702	−614	34.9	16.7	4.4	13300	3800
Average surface winds	71492	14721	−618	34.7	16.8	4.4	13300	3800
Preferred model: deep winds	71492	14696.1	−587.5	23.0	16.4	4.4	13300	3800

[a] CMB refers to core-mantle boundary.

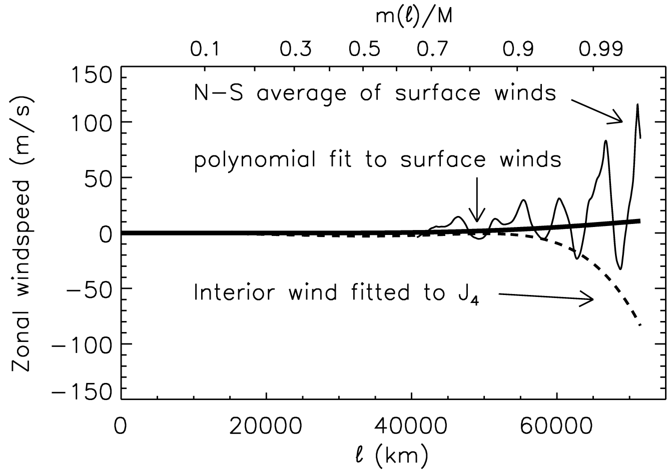

FIG. 4.—Jupiter's zonal wind speeds as a function of l, the distance from the rotation axis. The oscillating curve shows an average of northern and southern hemisphere surface zonal winds as determined by cloud motions; the heavy solid curve shows a fit of the surface winds with an eighth-order polynomial in l. The dashed curve shows our preferred rotation model that provides a match to Jupiter's low-degree gravitational moments with the DFT-MD EOS. The upper abscissa gives the relative mass enclosed within a cylinder of radius l.

2004). Because the mantle metallicity is so low, neither can we redistribute mass by invoking composition gradients. It is more plausible that Jupiter's J_4 is affected to a measurable extent by zonal winds in this pressure range. We bring the calculated J_4 into agreement without appreciably changing any other parameters of the model by assuming the zonal wind profile shown in Figure 4 (preferred model in Table 1 with the EOS profile given in Table 2). The shallower part of the wind profile could be adjusted further to force better agreement with J_6, but such a refinement lies outside the scope of this paper. We note a recent paper (Anderson & Schubert 2007) that models deep zonal flows in Saturn by fitting gravity data.

To ensure that numerical errors do not play any role in the mismatch of J_4, we checked our calculations with the standard theory for rotationally distorted models (Zharkov & Trubitsyn 1978). The results agree well with the more accurate SCF method.

It has been shown (Hubbard 1999) that high-order Jupiter gravity harmonics are sensitive to interior dynamics in the outermost planetary layers at pressures less than about 10 GPa.

TABLE 2
EOS FOR OUR PREFERRED JUPITER MODEL

Equatorial Radius R_e (km)	Density (kg m^{-3})	Pressure (GPa)	Temperature (K)	Mass Fraction $M(R < R_e)/M_J$
12.598	3904.3	3764.3	13272	0.0519
41.322	2102.2	1034.0	8928	0.4562
61.490	788.3	107.1	4930	0.9212
63.934	596.9	57.5	4381	0.9585
66.990	345.4	18.9	3982	0.9887

NOTE.—Table 2 is published in its entirety in the electronic edition of the *Astrophysical Journal*. A portion is shown here for guidance regarding its form and content.

There is no significant uncertainty in the hydrogen EOS at these pressures, which are accessible to experiment (Nellis 2002). This is why we investigated whether the DFT-MD EOS, coupled with plausible models of Jovian mantle dynamics, could reproduce the observed Jovian gravity field. According to the Poincaré-Wavre theorem (Tassoul 2000), the requirement that there be a single pressure-density relation (barotrope) within Jupiter is a necessary and sufficient condition that deep wind speeds be constant on cylindrical surfaces of constant l. Mapping the observed wind speeds onto such cylinders and then fitting the implied centrifugal potential with a polynomial to degree eight in l, we obtain the heavy curve in Figure 4. When this fit is incorporated in the SCF calculations, we find insignificant shifts in the predicted values of J_n ($n = 2, 4, 6$), although the winds could affect higher order Jupiter gravity components (Hubbard 1999). The assumed retrograde deep zonal wind has negligible effect on Jupiter's total spin angular momentum, reducing the latter by only 0.06% with respect to a windless model.

New observational data for Jupiter are expected from the NASA mission *Juno*. This low-periapse orbiter will return unprecedented data on gravitational and magnetic fields during 2016. It may present the first direct evidence of deep interior zonal flows in Jupiter proposed here.

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REFERENCES

Anderson, J. D., Hubbard, W. B., & Slattery, W. L. 1974, ApJ, 193, L149
Anderson, J. D., & Schubert, G. 2007, Science, 317, 1384
Blöchl, P. E. 1994, Phys. Rev. B, 50, 17953
Boss, A. P. 2007, ApJ, 661, L73
Burrows, A., Hubeny, I., Budaj, J., & Hubbard, W. 2007, ApJ, 661, 502
Campbell, J. K., & Synnott, S. P. 1985, AJ, 90, 364
Chabrier, G., Saumon, D., & Potekhin, A. Y. 2006, J. Phys. A, 39, 4411
Delaney, K. T., Pierleoni, C., & Ceperley, D. M. 2006, Phys. Rev. Lett., 97, 235702
Fischer, D. A., & Valenti, J. 2005, ApJ, 622, 1102
Grevesse, N., Asplund, M., & Sauval, A. J. 2007, Space Sci. Rev., 130, 105
Guillot, T., Gautier, D., & Hubbard, W. B. 1997, Icarus, 130, 534
Guillot, T., et al. 2004, in Jupiter, ed. W. M. F. Bagenal et al. (Cambridge: Cambridge Univ. Press), 35
Hubbard, W. B. 1982, Icarus, 52, 509
———. 1999, Icarus, 137, 357
Hubbard, W. B., Slattery, W. L., & DeVito, C. L. 1975, ApJ, 199, 504
Johnson, K., & Ashcroft, N. W. 2000, Nature, 403, 632
Kresse, G., & Hafner, J. 1993, Phys. Rev. B, 47, 558
Lyon, S. P., & Johnson, J. D., eds. 1992, Los Alamos National Laboratory EOS Database, Report LA-UR-92-3407, Table Hydr5251
Mayer, L., Lufkin, G., Quinn, T., & Wadsley, J. 2007, ApJ, 661, L77
Militzer, B. 2005, J. Low Temperature Phys., 139, 739
Militzer, B. 2008, Phys. Rev. B, submitted (arXiv:0805.0317)
Mizuno, H. 1980, Prog. Theor. Phys., 64, 544
Nellis, W. J. 2002, Phys. Rev. Lett., 89, 165502
Nellis, W. J., et al. 1997, J. Chem. Phys., 107, 9096
Niemann, H. B., et al. 1998, J. Geophys. Res., 103, 22831
Perdew, J. P., Burke, K., & Ernzerhof, M. 1996, Phys. Rev. Lett., 77, 3865
Pollack, J., et al. 1996, Icarus, 124, 62
Ross, M., Ree, F. H., & Young, D. 1983, J. Chem. Phys., 79, 1487
Saumon, D., Chabrier, G., & Horn, H. M. V. 1995, ApJS, 99, 713
Saumon, D., & Guillot, T. 2004, ApJ, 609, 1170
Seidelmann, K. P., ed. 1992, Explanatory Supplement to the Astronomical Almanac (Sausalito: University Science Books)
Tassoul, J.-L. 2000, Stellar Rotation (Cambridge: Cambridge Univ. Press)
von Zahn, U., Hunten, D. M., & Lehmacher, G. 1998, J. Geophys. Res., 103, 22815
Vorberger, J., Tamblyn, I., Bonev, S., & Militzer, B. 2007a, Contrib. Plasma Phys., 47, 375
Vorberger, J., Tamblyn, I., Militzer, B., & Bonev, S. 2007b, Phys. Rev. B, 75, 024206 (and references therein)
Wong, M. H. et al. 2004, Icarus, 171, 153
Zharkov, V. N., & Trubitsyn, V. P. 1978, Physics of Planetary Interiors (Tucson: Pachart Publishing House)