Electrical and Thermal Conductivity of High-Pressure Solid Iron

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We study the electrical and thermal conductivity of iron at high pressures using time-dependent density functional theory. In doing so, we particularly consider the impact of a Hubbard correction (+U) specifically for regions where strong electron correlations are present. Using the TDDFT+U methodology, we examine the anisotropy in the thermal conductivity of HCP iron, which may provide insights into the transport properties at conditions relevant to the core-mantle boundary and the interior of the Earth.

I. INTRODUCTION

The properties of elemental iron under high pressure are of great interest due to its prominence in Earth’s core [1][4]. Two solid phases of iron have been broadly studied. Under ambient conditions, the stable structure of iron is a single-atom body-centered cubic (BCC) cell. At room temperature and pressures relevant to Earth’s core (360 GPa) [5][6], a single-atom hexagonal close-packed (HCP) cell appears to be the stable structure [7][8]. The phase boundary between the two phases relies on the knowledge of magnetic ordering in the BCC phase. Ferromagnetic BCC is the energetically favored ground state compared to paramagnetic BCC requiring spin-polarization to be taken into account [9]. Electronic correlations are significant in iron, but become less significant under pressure because the electronic kinetic energy increases more rapidly than the potential energy. Experiments using x-ray magnetic circular dichroism and x-ray absorption spectroscopy indicate a BCC-HCP transition [10][11] between 12-18 GPa. The disappearance of the net magnetic moment indicates the HCP phase is non-magnetic [12]. As the pressure increases, 3d electrons delocalize further and form hybridized 3d-4p states. This goes along with a reduction in magnetic moment [13]. Material properties are commonly modeled using density functional theory (DFT) [14][15]. While successful, strict semi-local approximations typically fail to capture even the qualitative physics of strongly correlated materials. However, methods that incorporate a Hubbard correction (DFT+U) for the on-site Coulomb interaction have found great success in computing the structural and electronic properties of these challenging material systems [16][17]. Dynamical mean field theory (DMFT)+DFT is an alternative approach for augmenting conventional DFT, which treats electronic correlations differently [18][19]. The standard approach for computing the electrical conductivity uses the Kubo-Greenwood (KG) formula [20][21]. Commonly, it is evaluated on Kohn-Sham orbitals, eigenvalues, and occupation numbers. The electrical conductivity in number of applications including strongly coupled plasmas [22][24] and liquid metals [25][28] was calculated with this method. However, using Kohn-Sham quantities in the KG formula amounts to neglecting the interaction kernel needed to capture collective effects are other features relevant to electronic excitations that determine transport properties [29]. A feasible alternative that describes electronic excitations more accurately is time-dependent DFT (TDDFT). Electrical and thermal conductivity are obtained as the linear response of the system with respect to an electric field. The standard procedure is to use linear-response TDDFT (LR-TDDFT) which yields the interacting response function by way of an interaction kernel that includes electron correlations in terms of the Hartree and exchange-correlation (XC) kernel. The utility of LR-TDDFT for computing full wavenumber and frequency resolved transport properties has been assessed comprehensively for solid [30] and liquid aluminum [31]. An alternative procedure is real-time propagation in time-dependent density functional theory (RT-TDDFT) [24][32][33]. This method yields the time-dependent physical current as the linear response of the system with respect to an electric field from which the electrical conductivity is obtained by directly simulating the microscopic form of Ohm’s law [34]. While TDDFT captures the transport properties of simple metals like aluminum quite well, its performance for less simple metals has not yet been established. DFT+U has been traditionally used in evaluating static properties, but the Hubbard correction has not yet been included in the TDDFT calculations of dynamical properties such as the electrical conductivity. In this work, we evaluate the electrical conductivity of BCC and HCP iron using both flavors of TDDFT under high pressure. We particularly include the effects of strong correlations in terms of a Hubbard correction and assess its significance. Additionally, we compute the thermal conductivity of HCP iron and its anisotropy under high pressure up to the conditions prevalent in the core-
mantle boundary of Earth’s interior. Furthermore, we demonstrate agreement of our TDDFT+U calculations with the experimental measurements reported by Ohta et al. 35.

II. METHODOLOGICAL AND COMPUTATIONAL DETAILS

Ground state DFT calculations of the equation of state (EOS) and initial Kohn-Sham orbitals are performed using the full-potential linearized augmented-plane wave code implemented in Elk 36. A k-point grid of 20 × 20 × 20 points and 16 × 16 × 16 points up to 60 bands per atom are considered for the BCC and HCP phases, respectively in a unit cell. A larger number of bands is especially required for LR-TDDFT calculations. The c/a ratio is fixed to 1.60 throughout for HCP in the experimental range 37–39. The Perdew-Burke-Ernzerhof (PBE) 40 exchange-correlation (XC) functional is used. The calculations with the Hubbard U are also carried out with spin-polarized PBE around the mean-field form with double counting 17,42 with an enhanced description of magnetic and structural properties (see Table 1 in the Supplemental Material 43). The Hubbard parameters (U = 0.125 Ha and J = 0.033 Ha) used in this work are well-tested for high-pressure iron 37,44 and in the range used in earlier studies of ambient iron 17. 

LR-TDDFT calculations are performed by setting the exchange-correlation kernel to zero (f_{XC} = 0) which is referred to as the random phase approximation (RPA) in the LR-TDDFT formalism. Including a non-zero XC kernel based on commonly used XC approximations does not seem to have a significant impact on electronic transport properties 31. The LR-TDDFT calculations are performed with a fixed energy resolution set to 0.07 mHa. RT-TDDFT 45 and the methodology to extract the electrical conductivity from the microscopic form of Ohm’s law are described in Ref. 34. Also, note that we use Hartree atomic units everywhere in the parameters for TDDFT calculations. Within the RT-TDDFT calculations, a sigmoidal pulse of vector amplitude 0.1 a.u. is applied with a peak time of 2 a.u. having a full-width half maximum (FWHM) of 0.5 a.u. for a total simulation time up to 2000 a.u. (1 a.u. = 24,819 attoseconds) providing an energy resolution up to ~0.07 mHa in frequency space.

III. RESULTS

A. Equation of State

The pressure-volume curve shown in Fig. 1 is obtained by fitting total energies from DFT calculations using the PBE functional (GGA) 40 for various volumes to the Vinet equation of state (EOS) 46,47. The calculations with a Hubbard U are also carried out for the spin-polarized case using the PBE functional around the mean-field form with double counting 17,42. Our new work are indicated by the red lines in Fig. 1. 

In the BCC phase, the improvement of GGA+U over just using a GGA functional is rather small but still significant. A clear shift towards an agreement with the experimental results of Dewaele et al. 48 are achieved by the GGA+U calculations. They are also in agreement with the LDA calculations that are enhanced by dynamical mean field theory (DMFT) calculations by Pourvoskii et al. 49. However, our results indicate that using a GGA functional is sufficient for capturing the ground state properties 17 of the ferromagnetic BCC phase reasonably well taking into account the large static exchange splitting. 

With increasing pressure, antiferromagnetic HCP 50–52 is the stable phase (~13 GPa onwards, see Fig. 3 in the Supplemental Material 43 for the enthalpy curve). Here, electron correlations are more significant, because the static exchange splitting reduces bonding. In prior work, these dynamical many-body effects have been taken into account using DMFT 53 (see Fig. 2 in the Supplemental Material 43 for the effect of +U on the density of states). In the HCP phase, we notice a similar trend as in the BCC phase. At lower pressures, HCP iron is strongly correlated. While our GGA results match well with the available DFT and quantum Monte Carlo (QMC) data in the literature 39,48,51,53, they differ visibly from the experimental data. Consequently, our GGA+U calculations yield more accurate results and are in agreement with the LDA+DMFT results of Pourvoskii et al. 49 between 13-30 GPa. But even by ostensibly improving the treatment of strong correlations due to the Hubbard correction, the volume change in the EOS still deviates from the experimental data 54,55,60 by ~5% at ~70 a.u.³/atom. GGA predicts a c/a ratio of less than 1.60 which further reduces with increasing volume 53, while DMFT predicts a nearly constant c/a ~ 1.60 with change in volume in agreement with the experimental measurements 7,37,53 At pressures 40-50 GPa, the correlations are slightly better captured by LDA+DMFT compared to GGA+U. At higher pressures (>100 GPa), our GGA results are in good agreement with the experiments 17,56,59 and previous theoretical efforts 39,51,60 as correlations become less important.

B. Dynamical Conductivity

1. BCC Iron

The frequency-dependent conductivity $\sigma(\omega)$ of BCC iron under ambient conditions obtained using LR-TDDFT and RT-TDDFT both with Hubbard corrections is shown in Fig. 2. We compare our results with the KG results by Alfè et al. 61, which are available at a slightly ele-
vated temperature (T=500 K), and experimental results by Paquin [62], Palik [63] and Cahill [64]. Overall, the RT-TDDFT results are in best agreement with the experimental results by Paquin [62] and Palik [63], and LR-TDDFT with the experimental results by Cahill [64] up to 25 eV. KG and LR-TDDFT do not provide an accurate description across the entire frequency domain. Furthermore, KG completely misses the feature at ~55 eV albeit a slight peak-like increase in structure at ~50 eV. Nevertheless, KG has been shown to capture this strong feature in the dynamic structure factor of iron at much elevated temperatures [63]. LR-TDDFT essentially performs better than KG across the considered frequency range. This is due to the inclusion of local-field effects in the dielectric function [65, 66]. Furthermore, LR-TDDFT is still in good agreement with RT-TDDFT at higher frequencies, i.e., >60 eV.

The peaks near 55 eV and 90 eV seen in this work have been a subject of interest to characterize bound-bound transitions involving 3p, 3s and 3d orbitals in iron at elevated temperatures [63]. The effect of the Hubbard correction is negligible across the higher frequency range as expected since a shift in the electronic structure is mainly expected for the 3d electrons. However, the Hubbard correction causes a slight blueshift and an increased broadening of the peak near 50 eV seen in both LR-TDDFT and RT-TDDFT results (see Fig. 1 in the Supplemental Material [65]).

All the considered methods approach the DC conductivity (ω → 0) indicated by arrows in the inset plot in the range 8.63 MSm⁻¹ to 9.03 MSm⁻¹ close to the reported values in experiments [67, 68]. The DC value for KG results are extracted from a Drude-like fit to a restricted set of low-energy spectra for various k-point sampling and cell sizes [61]. With the inclusion of +U, RT-TDDFT and LR-TDDFT yield nearly identical DC conductivity.

It is common to verify simulation data in terms of the $f$-sum rule [69]

$$\frac{1}{\pi} \int_{0}^{\infty} d\omega \sigma(\omega) = n_e,$$  \hspace{1cm} (1)

where $n_e$ is the number of electrons in the simulation cell. Evaluated in a frequency range up to ~5 Ha (i.e., ~136 eV) and normalized to the $f$-sum rule of the experimental data by Paquin [62], this yields ratios of 0.95 for RT-TDDFT and 0.99 for LR-TDDFT, compared to 0.97 using KG formula obtained by Alfé et al. [61] evaluated up to ~5.5 Ha (i.e., ~150 eV directly from the $f$-sum rule) providing a measure of the quality of our calculations.

2. HCP Iron

In the HCP phase, we evaluate the conductivity tensor similar to the BCC phase discussed earlier but along various directions and analyze the corresponding tensor components. This is relevant because the asymmetrical HCP lattice ($a = b \neq c$), as opposed to the BCC lattice, requires computation of additional tensor components and could be of great aid for characterizing materials exhibiting the Hall effect [70, 71]. Fig. 3 shows the frequency-dependent conductivity of HCP iron at 23 GPa obtained using RT-TDDFT and LR-TDDFT with +U corrections along the directions $\bar{Z}$ (top panel) and $\bar{X}$ (bottom panel). There are currently no experimental or theoretical data available to be compared at these conditions, hence our work provides the first benchmark to be tested in future experiments. LR-TDDFT results are in good agreement with the RT-TDDFT results up to 55 eV along both the
FIG. 3. Dynamical electrical conductivity of HCP iron at 23 GPa computed using LR-TDDFT and RT-TDDFT with Hubbard $U$ corrections along directions $\hat{Z}$ (top panel) and $\hat{X}$ (bottom panel). Anisotropy in the DC conductivity is inferred from the arrows in the inset plots.

directions. With LR-TDDFT, a peak structure similar to the case of BCC is observed around 55 eV where RT-TDDFT yields a step increase in conductivity instead of a peak. Ignoring $+U$ corrections results in an increased broadening of the peak near 55 eV for the LR-TDDFT results similar to the case of BCC.

The inset plots show the minor differences at low frequencies and the associated DC conductivity indicated by arrows. Along the $\hat{Z}$ direction, we obtain DC values in the range 5.81 MSm$^{-1}$ to 7.42 MSm$^{-1}$ using LR-TDDFT and RT-TDDFT, respectively, which are in the range of experimental resistivity (inverse of conductivity) measurements [67, 68]. Along the $\hat{X}$ direction, the DC values are in the range 1.65±0.38 MSm$^{-1}$ to 4.76 MSm$^{-1}$ using RT-TDDFT and LR-TDDFT, respectively.

C. DC Conductivity with Pressure

Now we turn to the DC conductivity evaluated using RT-TDDFT at high pressures. Fig. 5 shows the DC conductivity as a function of pressure in the BCC and HCP phases at ambient temperature ($T=300$ K). The results in the BCC phase are indicated by solid red triangles and those in the HCP phase by empty red triangles. The error bars shown in our work are a result of post-processing and total time-propagation considered in the simulations (see Fig. 5 in the Supplemental Material [43]).

In the BCC phase, our predicted DC conductivity is in the range reported by several experiments [62, 63, 67, 72]. With increasing pressure in the BCC phase, the DC conductivity drops in agreement with the experiments [67, 68, 73, 74], and a drop in the conductivity is observed near 13 GPa which marks the transition between the BCC and the HCP phase. Note that a similar drop in the conductivity during the phase transition has been observed for several other materials [75, 76]. In contrast to the experimental results [67, 68, 73, 74] and our results, ab-initio calculations by Sha et al. [60] report an increase in the conductivity for the BCC phase with pressure although the drop in the conductivity during the phase transition is captured.

In the HCP phase, there is sufficiently good agreement between our results and experiments. They are in between Seagle and Gomi et al. [67, 68] up to 50 GPa and then in good agreement with Gomi et al. [67] for higher pressures. The black dotted line is a fit to the measurements on HCP iron by Zhang et al. [77] which is also in good agreement with our results up to 90 GPa. Our results are a lot lower than calculations by Sha et al. [60] who overestimate the conductivity in the HCP phase. The black dashed line shows the model based pressure and temperature dependence of the resistivity (inverse of conductivity) for the HCP phase derived by Seagle et al. [68] which is in good agreement with our results within the error bars at pressures above 50 GPa.

D. Thermal Conductivity in HCP Iron with Pressure

Finally, we compute the electronic component of the thermal conductivity of HCP iron versus pressure along the $\hat{Z}$ (top panel) and $\hat{X}$ (bottom panel) directions shown in Fig. 5. The thermal conductivity is computed from the electrical conductivity using the Wiedemann-Franz law. We use the ideal Lorenz number (2.44×10$^{-8}$ WΩK$^{-2}$) as its deviation is minimal at ambient temperature compared to high temperatures [29, 81].

Starting from the top panel, our results are in good agreement with the experimental data from laser-heated diamond anvil cell (DAC) measurements by Ohta et al. [35] for pressures less than 50 GPa. Our results with $+U$ corrections are indicated by right filled triangles, whereas those without by left triangles. The $+U$ corrections are particularly relevant at lower pressures where electronic correlations are more pronounced. When the $+U$ corrections are ignored, our results are still within the error bars of the experiment, but a deviation of up to 40% are observed along $\hat{Z}$ around 13 GPa. At higher
pressures (>50 GPa), we ignore the Hubbard corrections and extend the calculations up to the pressure regime found in the core-mantle boundary (CMB) in Earth’s interior (P~135 GPa, T~1000 K). Here, the reported thermal conductivity based on the bulk measurements by Ohta [79] and Zhang et al. [77] and the corresponding corrections arising due to sample thinning in DAC obtained by Lobanov et al. [80] are additionally shown in Fig. 3. At the core-mantle boundary conditions (P~135 GPa), we report κ_{Z}/κ_{X} = 3.03 ± 0.37 comparable to 2.56 ± 0.48 estimated by Ohta et al. [79]. The thermal conductivity of pure iron at core-mantle boundary conditions is estimated by Seagle et al. [68] to be 145 Wm^{-1}K^{-1}. This is in the range of our predictions, which is 157.8 ± 26.3 Wm^{-1}K^{-1}, and also of previous theoretical efforts [20, 82]. Additionally, the thermal conductivity measurements (bulk) at ambient temperature (T=300 K) by Hsieh et al. [83] are compared to the electronic contribution to the thermal conductivity evaluated using RT-TDDFT (diagonal components and trace averaged, see Fig. 4 in the Supplemental Material [43]). The total thermal conductivity including the magnetic and lattice components could be further individually resolved as demonstrated in the recent work by Nikolov et al. [84] with the leading contribution especially at ambient temperature stemming from the electronic component [85]. While taking into account the trace average of the conductivity tensor, the resulting thermal conductivity near core-mantle boundary conditions (P~135 GPa) is ~87 Wm^{-1}K^{-1}.

**IV. CONCLUSIONS**

In this work, we presented TDDFT+U results on the electrical and thermal conductivity of iron at high pressures. The inclusion of +U corrections are found to be crucial in the description of these properties, even at high pressures found in the Earth’s core [33]. This work presents a case for the importance of accurate calculations of electronic transport properties with TDDFT including Hubbard corrections. In the future, this can be used for studying the structural phase transitions and the spin response of materials under extreme conditions that become accessible with recent progress in free-electron lasers [77, 88]. The frequency-dependent electrical conductivity along with the case of anisotropy presented for HCP iron could serve as a benchmark for...
future experiments with special focus on advanced diagnostics. Magnetism has been shown to play a key role in iron-nickel alloys at Earth-core conditions stressing the importance of nickel which was previously assumed to be low [89]. Future research should examine the thermal conductivity anisotropy of iron along with nickel and other light elements at the actual core conditions of the Earth in order to provide more precise constraints on the thermal evolution and dynamics of Earth’s core and mantle. It may have significant effects on the evolution and dynamics of the Earth’s inner core if the thermal conductivity anisotropy in HCP iron is preserved at those conditions. Also the discrepancy in the experimentally determined electrical and thermal conductivity [79, 90] of iron at the conditions of Earth’s core could be answered by taking the anisotropy into account.

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