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Influence of oxygen on electronic correlation and transport in iron in the Earth's outer core

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Germán G. Blesio ^{® 1,2} ⊠, Leonid V. Pourovskii^{3,4}, Markus Aichhorn ^{® 5}, Monica Pozzo ^{® 6,7,8}, Dario Alfè ^{® 6,9} & Jernej Mravlje ^{® 1,10}

Knowing the transport properties of iron at the Earth's core conditions is essential for the geophysical modeling of Earth's magnetic field generation. Besides by extreme pressures and temperatures (which cause scattering by thermal disorder to dominate), transport may be also influenced by the presence of light elements and electron-electron scattering. We used a combination of molecular dynamics, density functional theory, and dynamical mean-field theory methods to examine the impact of oxygen impurities on the electronic correlations and transport in the Earth's liquid outer core. We find electronic correlations to be moderately enhanced by oxygen admixture. At realistic 10 atomic% of oxygen, the thermal conductivity suppression by electronic correlations (about 20%) is of the same magnitude as that due to oxygen inclusion. Hence, both play an equally important role in reducing the conductivity and stabilizing the geodynamo. We also explain the reduction of Lorenz ratio in core matter.

The Earth's magnetic field is generated by a self-excited dynamo, driven by convection processes within the outer core. Specifically, thermal convection plays a crucial role but is effective only if the total heat extracted at the core–mantle boundary surpasses the amount transferred through thermal conduction. Therefore, for geophysical models of the geodynamo mechanism, the thermal and electrical conductivities of the iron-rich alloys that make up the outer core are essential parameters. Direct measurements of transport under extreme pressures and temperatures that are relevant to Earth's core are challenging^{1,2} as one must ensure homogeneous temperature and accurately measure the geometry of the samples³.

One can assess transport properties also from first principle calculations based on the molecular dynamics (MD)-density functional theory (DFT) method^{4–6}. These calculations have shown that the electrical and thermal conductivities have values that are significantly (2–3 times) higher^{5,6} than earlier established estimates^{7,8}. These earlier estimates were based on extrapolations from conditions far from those experienced in the Earth's core and also neglected the effects of resistivity saturation^{9–11}. The higher values of thermal conductivity lead to a different geophysical picture, with an inner core that is younger (<1 billion years, whereas magnetism is known to exist for at least 3.4 billion years¹²⁻¹⁴), and less thermal convective energy to drive the geodynamo. This has come to be known as the new core paradox¹⁵. Namely, less thermal energy implies that convection must be helped by chemical convection driven by the exsolution of lighter elements as the inner core freezes, but this was less active before its formation. Recently, alternative exsolution mechanisms have been proposed, whereby MgO¹⁶ or SiO₂¹⁷ would precipitate out of the core as its temperature is reduced on secular cooling and the solubility of these light elements drops.

There has been an ongoing discussion on whether electronic correlations, which have been shown to be important in iron under Earth's core conditions^{18,19}, can cause a breakdown in the Mott–Ioffe–Regel resistivity saturation^{9,20}. This debate revolves around whether the correlations reduce the conductivity enough to resolve the core paradox^{21–23}, as suggested in a pioneering work²¹ (later retracted²⁴). Recent findings indicate that electron–electron scattering (EES) plays only a moderate role and represents

¹Jožef Stefan Institute, Jamova 39, Ljubljana, SI-1000, Slovenia. ²Instituto de Física Rosario (CONICET) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Rosario, Santa Fe, 2000, Argentina. ³CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, Palaiseau, 91120, France. ⁴Collège de France, Université PSL, 11 place Marcelin Berthelot, Paris, 75005, France. ⁵Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, Petersgasse 16, Graz, 8010, Austria. ⁶Department of Earth Sciences and London Centre for Nanotechnology, University College London, Gower Street, London, WC1E 6BT, UK. ⁷Institute for Materials Discovery, UCL East, Marshgate Building, 7 Sidings Street, London, E20 2AE, UK. ⁸Faculty of Technological & Innovation Sciences, Universitas Mercatorum, Piazza Mattei 10, Rome, 00186, Italy. ⁹Dipartimento di Fisica Ettore Pancini, Università di Napoli Federico II, Monte S. Angelo, Napoli, I-80126, Italy. ¹⁰Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, Ljubljana, SI-1000, Slovenia. ^[]e-mail: blesio@ifir-conicet.gov.ar

a small fraction compared to thermal-disorder (electron-phonon) scattering^{25,26}. Very recently, time-dependent density functional theory calculations found higher values of conductivity²⁷ compared to the ones obtained from the Kubo–Greenwood formula, which suggests that vertex corrections²⁸ may play a non-negligible role as well.

One important question remains to be addressed: does alloying with lighter elements significantly enhance correlations, and if so, to what extent are conductivities suppressed? The Earth's core contains a sizable fraction of lighter elements, believed to be primarily silicon and oxygen, with recent research indicating a high oxygen concentration²⁹⁻³². The influence of these substitutions has been broadly investigated using MD-DFT^{5,6,33,34} without accounting for correlation effects. Previous work²⁶ investigated Fe-Si alloys within DMFT, treating local electronic correlations with a perturbative weak-coupling approach. They found the correlation effects to be much smaller than the effects of the disorder with Si admixture strongly reducing EES contribution to resistivity. One could expect alloying with oxygen to enhance electronic correlations by reducing the iron 3d shell occupancy toward half-filling³⁵ and, correspondingly, to enhance the EES contribution to transport. Indeed, recent theoretical work³⁶ modeled the Fe-O phase at core conditions with hexagonal ordered Fe-O structures and found, in contrast to the Fe-Si case, a strong enhancement of EES with the fraction of EES in both electrical and thermal resistivity rapidly increasing with oxygen concentration. The impact of the thermal disorder on EES was neglected in that study, and the final effect on the thermal conductivity, taking into account both EES and electron-phonon scattering, was not evaluated. Furthermore, the impact of EES on the conductivity in liquid iron, which is highly relevant for the dynamo mechanism, was not clarified.

Here we investigate the transport properties of Fe and Fe–O alloys in their liquid state at inner-core boundary (ICB) and core-mantle boundary (CMB) conditions. To include the effects of the compositional disorder, lattice disorder, and electronic correlations on equal footing, we combine an MD-DFT description of liquid atomic dynamics and electron-lattice scattering with dynamical mean-field theory (DMFT) and a quantum Monte Carlo treatment of electronic correlations^{23,25,37–39}. We focus on a Fe_{0.91}O_{0.09} composition and observe that its EES rate increases by ~20% compared to pure iron (Fe). The electrical and thermal conductivities drop by ≈10% and ≈20%, respectively. We find that the thermal disorder remains the main source of scattering, and we interpret the reduction of conductivities in terms of compositional disorder-induced changes in the band-dispersion (containing both direct effects of impurity potential and modification of vibrational patterns) rather than a direct increase in EES.

In order to quantify the effects of electronic correlations on transport, we compare the calculated DMFT conductivities with those from MD-DFT at the same compositions. We find that the inclusion of EES leads to a moderate but non-negligible reduction of electrical and thermal conductivities by roughly 10% and 20%, respectively (thus an equal amount to the just quoted reduction due to oxygen inclusion). This finding is crucial considering a large body of existing theoretical work that neglects EES^{5,6,11,33}. The fraction of EES in both electrical and thermal Fe–O resistivity in our calculations that do not assume Matthiessen's rule²⁵ remains the same as in pure iron in contrast to the earlier result³⁶.

We discuss why the thermal conductivities are suppressed more than the electrical ones and highlight the geophysical implications of our results.

Results

We calculate the liquid phase for 67 and 157 atoms: all iron (Fe) or with oxygen (Fe_{0.91}O_{0.09}). We study the liquid at CMB conditions for a temperature T = 4400 K, volume 8.64 Å³/atom (which corresponds to pressure 132 GPa), and ICB conditions T = 6350 K with volume 7.16 Å³/atom (pressure 330 GPa).

The results below are for 67 atoms supercells, which were performed for three snapshots separated by 5 ps, and the transport quantities were obtained by averaging over the snapshots and spatial directions. We show the comparison with the 157 atoms calculations that demonstrates the convergence with respect to the supercell size in Fig. SI2 in Supplementary Information.

Electronic correlations

Figure 1 displays the imaginary part of self-energies for a single snapshot in the energy range of [-1, 1] eV. Each curve represents a different site/orbital/ spin index, and the thick lines indicate an average over all of them. Since the EES rate is $1/\tau = -2Im\Sigma(\omega \rightarrow 0)$, more negative values of Im Σ indicate stronger electronic correlations (see Fig. SI1 in Supplementary Information). The correlations are overall stronger at the CMB; the impact of bandwidth reduction that leads to an enhancement of correlations with increasing volume overweights the electronic scattering increases notably in the oxygen-rich case, both at the ICB and at the CMB. The distribution of the curves reveals that not only the Fe sites closest to oxygen are affected, but also that the spread of the data is wider in the oxygen-rich case, and even the self-energies with the smallest magnitudes are enhanced by oxygen. Overall, the average EES, as given by the average Im Σ , increases by 20%.

Conductivities

The calculated optical conductivities are shown in Fig. 2 for the case of electrical and thermal current in the top and bottom panels, respectively. The $\omega \rightarrow 0$ values indicate the dc-transport values. One sees that quantitatively the effect of oxygen on transport is somewhat weaker than on the EES. Also shown in that figure are the results of a simplified calculation where one uses the $\langle \Sigma \rangle$ instead of the individual self-energies. One sees a "self-averaging" effect: the results of such a calculation are almost indistinguishable from the full calculation. This also shows that statistical uncertainties of the individual self-energies will not affect the calculated conductivities.

To what extent is the suppression of conductivities in the oxygen-rich case due to the increase of EES documented in Fig. 1? It turns out that, as suggested in the earlier work²⁵, iron under Earth's core conditions is in a thermal-disorder-dominated case where the changes of EES impact transport weakly. In Fig. 3, we demonstrate this by additional calculations where we compute the conductivity of the $Fe_{0.91}O_{0.09}$ case by using EES



Fig. 1 | Imaginary part of the self-energies. Imaginary part of the calculated selfenergies on the real axis. In the top and middle panels, we show the individual selfenergies (blue lines) and their average $\langle Im\Sigma \rangle$ (black thick). In the bottom panel, the four average self-energies are shown, at the ICB (full) and CMB (dashed) conditions.



Fig. 2 | **Optical and thermal conductivity.** Optical electrical (top) and thermal (bottom) conductivity for pure Fe and $Fe_{0.91}O_{0.09}$. The ICB and CMB cases are shown on the left and right, respectively. The dashed lines (that overlap closely with





Fig. 3 | **Self-energies effect in** $\kappa(\omega)$. Thermal conductivity for pure Fe and Fe_{0.91}O_{0.09} for the ICB (top) and CMB cases (bottom). We show the results obtained with orbitally and site-resolved self-energies (dots) as well as those calculated using the average self-energy (full line). The latter was first averaged over all sites and orbitals on the Matsubara grid and then analytically continued. The differences between the two are very small. With dash-dotted line, we show results calculated by exchanging the average self-energy between the Fe and Fe_{0.91}O_{0.09}.

corresponding to pure Fe calculation and vice versa for the other case. Quite strikingly, these "exchanged" calculations are at small frequencies almost indistinguishable from the "non-exchanged" ones. This shows that oxygen affects the results through a structurally induced change in the band dispersions (containing both the direct effect of impurities on electron motion and the indirect effect via the modifications of Fe displacements) and that the changes in the EES play an insignificant role. This is further demonstrated in Fig. SI3 in Supplementary Information where the scattering is artificially increased, and only a weak effect on transport is seen.

Figure 4 shows the calculated values of resistivity (top) and thermal conductivity (bottom) along with data from the literature. Thermal disorder dominates: perfect crystalline lattices have much higher conductivities ($\kappa \sim 500 \text{ W m}^{-1}\text{K}^{-1}$, $\rho \sim 20 \,\mu\Omega \text{ cm}$) outside of the range of the plot. Inclusion of EES clearly has less effect but is not negligible: it is seen to change the results to a similar extent as the inclusion of the oxygen at the 10% level. The results from the literature that neglects EES coincide with ours only at a higher (25%) oxygen level. On the other hand, we notice that calculations based on ordered structures (brown) overestimate the effects of EES.

Suppression of Lorenz ratio

Interestingly, EES suppresses the thermal conductivities more than the electrical ones. Figure 5 shows the evolution of the Lorenz number $L = \kappa / (\sigma T)$ with respect to the strength of EES, which is scaled by the factor α , as described in Supplementary Note 3. For pure Fe, the value of L due to electron–phonon scattering is almost identical to the standard value of 2.44×10^{-8} (W Ω K⁻²), whereas it is considerably reduced when EES is taken into account. This reduction occurs because inelastic EES affects κ more strongly than σ . Specifically, κ is determined by integrating $\Gamma(\omega)\omega^2(-df/d\omega)$, where $\Gamma(\omega)$ is the transport distribution function, *f* is the Fermi function, and ω is the frequency. On the other hand, σ is calculated by integrating $\Gamma(\omega)$ ($-df/d\omega$), which only involves the derivative of the Fermi function. The conductivity is mostly given by states around $\omega = 0$, while the dominant contribution to thermal conductivity occurs at finite energies $1.5 \text{ T} \leq |\omega| \leq 4 \text{ T}$.

The right panel of Fig. 5 presents the transport distribution $\Gamma(\omega)$ for the CMB case, which is evaluated for the actual EES (full) and compared to a calculation where the energy dependence of scattering is suppressed and the self-energy Im $\Sigma \rightarrow$ const is taken (dashed), corresponding to a DFT transport distribution. It is evident that the increase of EES with energy suppresses Γ that becomes smaller at larger energies compared to the DFT transport distribution case. Additionally, a comparison between Fe and Fe–O is interesting, which is evident from the DFT transport distributions. The inclusion of oxygen leads to notable suppression of transport

distribution at $\omega = 2.5$ eV, caused by O–2*p* hybridization with the 4s iron states. This explains the smaller Lorenz number in the oxygen-rich case.

Discussion

In summary, our study focused on the impact of oxygen on electronic transport in liquid iron at Earth's outer core conditions. Because oxygen diminishes the Fe 3*d* electronic occupation towards half-filling, it can be expected to enhance electronic correlations. We indeed find that the EES is



Fig. 4 | Results of resistivity and thermal conductivity in the context of literature. Resistivity (top) and thermal conductivity (bottom) for Fe and Fe_{0.91}O_{0.09} for the ICB and CMB cases calculated using DMFT (including both electron–electron and e.–ph scattering) and DFT (e.–ph. only) are shown with full symbols. The results from previous works^{6,23,25,27,34,36,69} are also shown for comparison (open symbols and crosses) as well as solid phases calculated at ICB conditions^{23,25,36}.

Fig. 5 | Suppression of Lorenz ratio. (left) Lorenz number for Fe (bullets) and Fe_{0.91}O_{0.09} (crosses) and for the ICB (full line) and CMB cases (dashed line). We use the parameter α to artificially change the magnitude of the EES $\Sigma \rightarrow \Sigma_{\alpha} = \text{Re}\Sigma + \alpha i \text{Im}\Sigma$, with $\alpha = 1$ corresponding to the full DMFT calculation. One sees that the Lorenz number is reduced by the presence of oxygen. Results from literature^{6,34,69} are shown separately on the left with symbols and colors as in Fig. 4. These points correspond to a vanishing EES i.e., $\alpha = 0$. (right) Transport distribution $\Gamma(\omega)$. Solid curves the obtained from the full DMFT self-energy, dashed lines from a constant scattering rate approximation. moderately increased. The numerical values of the conductivities and the Lorenz ratio are given in Table 1. The oxygen substitution at ~10% level, which is a plausible content for the outer core, suppresses electrical (thermal) conductivities by about 10(20)% only. The electronic correlations suppress the conductivities to a similar extent as oxygen inclusion: for both Fe and Fe–O the suppression due to electronic correlations amounts to roughly 10(20)% for the electrical (thermal) conductivity, which is consistent with previous studies on iron in the inner core²⁵. In contrast to previous work³⁶, we find that the EES fraction in resistivity remains constant with oxygen admixture. Based on that and earlier findings²⁵, we propose that the reduction of thermal conductivity by 20% can, therefore, be used as a rule of thumb when direct calculations of EES are not feasible.

What are the geophysical implications of electronic correlations? The first observation is that their effect is moderate. The drastic reduction of conductivity, which was predicted on the basis of EES enhancement in ordered Fe-O structures³⁶, is not observed when thermal disorder effects are simultaneously included. But it is also clear from our study that one cannot neglect electronic correlations, since the reduction of conductivities due to EES is comparable to the reduction of conductivities caused by light elements (impurity scattering). Importantly, some models that assume a higher heat flow from the core find a thermally only driven geodynamo for κ below a limiting value that is of order 100 W $m^{-1}K^{-1}$ $^{40-42}$. EES, whereas small compared to the thermal disorder, might in the end provide just the necessary additional scattering next to the compositional disorder to power the geodynamo sufficiently. At the very least, whenever one argues that compositional disorder is important, EES must not be neglected either since our study shows that their respective contributions to conductivity are close in magnitude. Another important finding is the universal suppression of the Lorenz number: thermal conductivities are affected by EES more than electrical ones^{22,23}. This is seen to be also an effect of compositional disorder in the Fe-O case, but EES enhances this further by supressing the contribution of states away from the Fermi energy. This is important both to properly interpret the high-pressure measurements that mostly probe σ and for the geodynamo, because of the distinct influence of the two quantities there. Thus, these effects of EES must be taken into account for a proper understanding of terrestrial planetary interiors.

In future studies, it would be interesting to investigate also alloying with sulfur and silicon³³. Both elements affect the transport properties strongly at the DFT level because, unlike oxygen that alloys interstitially³³, they alloy substitutionally and, therefore, more strongly affect the bond disorder with perhaps different implications for electronic correlations. The silicon case was recently investigated²⁶, and the total thermal conductivity for CMB seems compatible with what we find at comparable concentrations of oxygen. However, a drastic reduction of the EES fraction in resistivity by Si reported in this work is qualitatively different from the picture we find for Fe–O. Additional DMFT studies evaluating the EES effect in the Fe–Si system, which does not entirely rely on perturbative many-body



Table 1 | Main results for Fe and Fe–O

	СМВ		ICB	
	<i>T</i> = 4400 K		<i>T</i> = 6350 K	
	V = 8.64 Å ³ /at		<i>V</i> = 7.16 ų/at	
Case	Fe	Fe-O	Fe	FeO
$-\mathrm{Im}\langle\Sigma(\omega=0) angle$ (eV)	0.11	0.14	0.09	0.11
$\sigma_{\rm DFT} (10^4 \Omega^{-1} {\rm cm}^{-1})$	1.35	1.24	1.54	1.37
$\sigma_{\rm DMFT} (10^4 \Omega^{-1} {\rm cm}^{-1})$	1.22	1.10	1.41	1.28
$1 - \sigma_{\text{DMFT}} / \sigma_{\text{DFT}}(\%)$	10	11	9	7
$\kappa_{\rm DFT} ({\rm W} {\rm m}^{-1} {\rm K}^{-1})$	145	120	243	190
$\kappa_{\rm DMFT}$ (W m ⁻¹ K ⁻¹)	119	99	193	158
$1 - \kappa_{\text{DMFT}} / \kappa_{\text{DFT}}(\%)$	18	17	21	17
$L_{\rm DFT} (10^{-8}{ m W}\Omega{ m K}^{-2})$	2.43	2.20	2.48	2.18
L _{DMFT} (10 ⁻⁸ W Ω K ⁻²)	2.22	2.05	2.16	1.95

Summary of results for CMB and ICB conditions, both for Fe and Fe0.91O0.09.

approaches, could be useful to understand the origin of this difference. Sulfur admixture that would act also in an oxidizing way could potentially have a bigger effect than Si. Whereas the sulfur concentrations are believed to be negligible on Earth⁴³, they are expected to be sizable in extraterrestrial planets^{44–46}. An important, technically very challenging aspect to be explored in future research is the possible influence of vertex corrections²⁸ that are neglected in this work and might lead to the increased conductivity found in time-dependent DFT studies²⁷. Finally, both thermal disorder and compositional disorder are also important for Fe oxides that are relevant for the properties of the lower mantle, where, for example, FeO is predicted to be^{47–50} in a state where electronic correlations are very strong, and the influence of thermal and compositional disorder might lead to large effects there.

Methods

We performed the MD-DFT calculations with the VASP code⁵¹ using the projected augmented wave method^{52,53} and PW91 exchange-correlation potential⁵⁴ to describe the interactions between the electrons and the ions and expanded the single-particle orbitals as linear combinations of plane waves (PW), including PW with maximum energies of 400 eV. The molecular dynamics simulations were performed by sampling the Brillouin zone using the Γ point only, and a time step of 1 fs. The temperature was controlled using the Nosé⁵⁵ thermostat. To compute the DFT electrical and thermal conductivity, we used the modified version of VASP by Dejarlais⁵⁶.

Snapshots of atomic positions obtained with MD-DFT were subsequently used as input for DFT+DMFT. Variability of the liquid structure is then included both in terms of considering supercells of sufficient size and by considering several snapshots. With the growing size of the supercell, the spatial variations within a single supercell represent the variability well, and the difference between results corresponding to distinct snapshots diminishes. In particular, we chose three liquid configurations at sufficiently separated times of 5 ps as input for the DFT + DMFT calculations.

The DFT + DMFT self-consistent calculations were performed with a local density approximation (LDA) approach in the Wien2K code^{57,58}, using the TRIQS library⁵⁹⁻⁶² for the DMFT and transport calculations. We used a local density-density interaction vertex with interaction parameters U = 5.0 eV, $J_{\rm H} = 0.93 \text{ eV}$. These values are in agreement with previous studies on pure iron^{22,23,25} and are supported by recent first-principles estimates finding *U* in the range of 4–5.5 eV in pure iron at ambient volume^{63,64} and its moderate enhancement by strong compression⁶⁵. We solved the impurity problem using the continuous-time hybridization-expansion segment solver^{66,67}. Each calculation was first converged by 25 fully self-consistent DFT+DMFT iterations, where each Monte Carlo run employed 2×10^{10} Monte Carlo moves and 200 moves/measurement. Using the converged Kohn–Sham Hamiltonian, 10 additional DMFT cycles were performed with

the number of Monte Carlo moves increased to 10^{11} . To obtain clean data for analytical continuation that we performed using the Maximum Entropy method, 20 additional runs (with 2×10^{11} moves per run) were carried out starting from the same converged value of the DMFT bath Green's function and resetting the random sequence.

We calculated the conductivities within the Kubo linear-response neglecting vertex corrections. The electrical and thermal conductivity ${\rm read}^{\rm 62,68}$

$$\sigma_{\alpha\alpha'} = \frac{e^2}{k_{\rm B}T} K^0_{\alpha\alpha'}, \kappa_{\alpha\alpha'} = k_{\rm B} \left[K^2_{\alpha\alpha'} - \frac{\left(K^1_{\alpha\alpha'}\right)^2}{K^0_{\alpha\alpha'}} \right],\tag{1}$$

where α is the direction (*x*, *y* or *z*) and *k*_B is the Boltzmann constant. The kinetic coefficients $K_{\alpha\alpha'}^n$ are

$$K_{\alpha\alpha'}^{n} = 2\pi\hbar \int d\omega (\beta\omega)^{n} f(\omega) f(-\omega) \Gamma^{\alpha\alpha'}(\omega,\omega), \qquad (2)$$

where 2 is the spin factor, $f(\omega)$ is the Fermi function, and the $\Gamma^{\alpha\alpha'}$ is given by

$$\Gamma^{\alpha\alpha'}(\omega,\omega') = \frac{1}{V} \sum_{\mathbf{k}} \operatorname{Tr}\left(\nu_{\mathbf{k}}^{\alpha} A_{\mathbf{k}}(\omega) \nu_{\mathbf{k}}^{\alpha'} A_{\mathbf{k}}(\omega')\right)$$
(3)

where *V* is the unit-cell volume, $A_{\mathbf{k}}(\omega)$ is the DMFT spectral function at momentum \mathbf{k} , and $\nu_{\mathbf{k}}^{\alpha}$ is the corresponding band velocity in the direction α . Additionally, we define the transport distribution

$$\Gamma(\omega) = \sum_{\alpha} \Gamma^{\alpha\alpha}(\omega, \omega).$$
(4)

We also calculated the response at a finite frequency Ω which yields the optical–electrical and thermal conductivity. These are evaluated by Eq. (1) using the kinetic coefficients evaluated at a finite frequency Ω

$$K^{n}_{\alpha\alpha'}(\Omega) = 2\pi\hbar \int d\omega \Gamma^{\alpha\alpha'}(\omega + \Omega/2, \omega - \Omega/2)(\omega + \Omega/2)^{n} \\ \beta^{n-1} \frac{f(\omega - \Omega/2) - f(\omega + \Omega/2)}{\Omega}.$$
(5)

In the momentum sums of Eq. (3), we retained 14 momentum points. The electron–phonon-only values were calculated using the Kubo–Greeenwood approximation as implemented in VASP⁵⁶ using 10 momentum points. We checked that upon increasing the number of momentum points further, the results vary by <1%.

Data availability

The datasets source of all figures are available in the Zenodo repository under accession code https://doi.org/10.5281/zenodo.10841624.

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Author contributions

G.G.B. carried out the DFT + DMFT electronic structure and transport calculations. D.A. and M.P. carried out the DFT molecular dynamics and transport calculations. G.G.B., J.M., L.V.P., M.A., and D.A. discussed the results and wrote the paper.

Competing interests

The authors declare no competing interests.

Additional information

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Correspondence and requests for materials should be addressed to Germán G. Blesio.

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