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# Impact of electronic correlations on the superconductivity of high-pressure CeH<sub>9</sub>

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Rare-earth superhydrides have attracted considerable attention because of their high critical superconducting temperature under extreme pressures. They are known to have localized valence electrons, implying strong electronic correlations. However, such many-body effects are rarely included in first-principles studies of rare-earth superhydrides because of the complexity of their high-pressure phases. In this work, we use a combined density functional theory and dynamical mean-field theory approach to study both electrons and phonons in the prototypical rare-earth superhydride CeH<sub>9</sub>, shedding light on the impact of electronic correlations on its critical temperature for phonon-mediated superconductivity. Our findings indicate that electronic correlations result in a larger electronic density at the Fermi level, a bigger superconducting gap, and softer vibrational modes associated with hydrogen atoms. Together, the inclusion of these correlation signatures increases the Migdal-Eliashberg superconducting critical temperature from 47 K to 96 K, close to the measured 95 K. Our results reconcile experimental observations and theoretical predictions for CeH<sub>9</sub> and herald a path towards the quantitative modeling of phonon-mediated superconductivity for interacting electron systems.

Pressure-induced metallic hydrogen stands as the holy grail of high-pressure physics, with a long belief in its potential room-temperature superconductivity<sup>1</sup>. Although the theoretical pathway is well-established, the experimental realization of metallic hydrogen is hindered by the ultra-high pressure required for metallization and the difficulty of probing samples under extreme conditions. A significant advancement in this field came with Ashcroft's proposal of *chemical pre-compression*<sup>2,3</sup>. This scheme widens the phase space in which a high-temperature superconductor can be found, ultimately leading to superhydrides that transition to a superconducting state at pressures lower than those predicted for elemental hydrogen<sup>4</sup>.

Among the various candidates, rare-earth metal superhydrides have shown great promise, especially with the discovery of LaH<sub>10</sub><sup>5–8</sup>. It exhibits a superconducting critical temperature of around 250 K at 170 GPa, marking the highest measured superconducting critical temperature to date. Furthermore, cerium superhydrides (CeH<sub>*n*</sub>, with *n* = 9 or 10) have also attracted attention: although their maximum superconducting critical temperatures do not exceed that of LaH<sub>10</sub>, they reach a relatively high superconducting critical temperature (around 100 K) at pressures on the order of 100 GPa or less<sup>9–11</sup>. This lower-pressure regime not only simplifies high-pressure synthesis and characterization but also further brings the goal of ambient-

pressure superconductivity closer to fruition. In general, numerous rare-earth superhydrides have been predicted and synthesized in the past decade<sup>5,9,12–20</sup>, but a pivotal yet unresolved question persists. What role do electronic correlations, induced by the *f*-electrons of the rare-earth elements, play in these high-pressure compounds? In LaH<sub>10</sub>, it has been observed that external pressure destabilizes the 6s- and 5d-orbitals of La, making the 4f-orbitals energetically more favorable<sup>21</sup>. As a result, the electronic states of LaH<sub>10</sub> near the Fermi level are composed of La 4f- and H 1s-orbitals<sup>22</sup>. We note that these states involving La 4f-orbitals are strongly localized and generally cannot be well described by density functional theory (DFT)<sup>23,24</sup>.

To gain insight into the question of the role of electronic correlation in rare-earth superhydride, we choose CeH<sub>9</sub> as a representative example and explore many-body effects using a combination method of DFT and dynamical mean-field theory (DMFT), known as DFT+DMFT<sup>25–33</sup>. Previous studies have shown that the strong correlation nature of cerium *f*-electrons plays a central role in the isostructural phase transition of cerium in its elemental form<sup>34–38</sup>, in cerium intermetallic compounds<sup>39,40</sup>, other rare-earth metals<sup>41,42</sup>, Kondo insulators<sup>43,44</sup>, as well as heavy-fermion systems<sup>45,46</sup>. We address the notable gap between the experimental results<sup>9–11,14</sup> and theoretical forecasts<sup>12,13,47</sup> regarding the critical temperature of phonon-

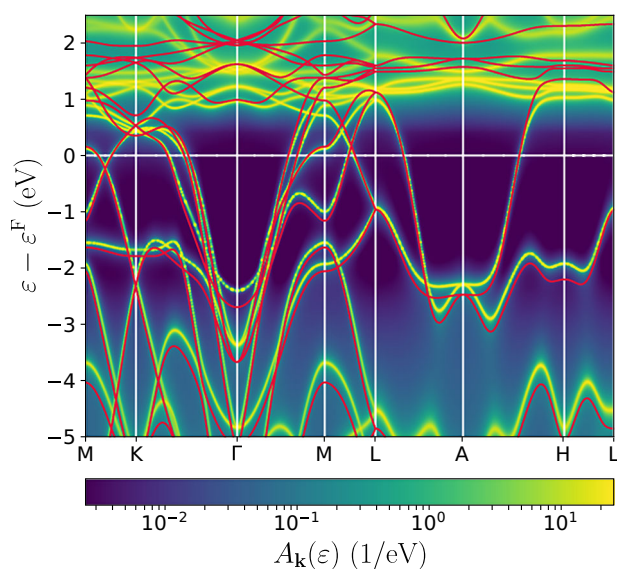
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mediated superconductivity in CeH<sub>9</sub> under high pressure. Theoretical calculations based on DFT underestimate the superconducting critical temperature by nearly 50%<sup>9</sup>, prompting speculation about the role of electronic correlations. Our work enhances the description of phonon-mediated superconductivity by incorporating electron-correlation effects for electronic and phononic interactions.

## Results

### Correlated electrons

We study the impact of electronic correlation effects in CeH<sub>9</sub> by comparing DFT results to DMFT many-body calculations with the nominal double-counting scheme<sup>37</sup>. To this end, we first obtain the crystal structure of CeH<sub>9</sub> from first principles by optimizing the internal atomic coordinates and the lattice constants of the crystal under 200 GPa using DFT, see Section S1 in the Supplementary Information (SI). Treating the Ce 4*f*-electron as valence electrons in the pseudopotential calculations is necessary to obtain lattice parameters in agreement with measurements<sup>48</sup>, suggesting that the Ce-4*f*-electrons, although being more closely bound, are not atomic-like. Turning to the electronic structure, we compare in Fig. 1 the DFT band-structure (red



**Fig. 1 | Comparison of the electronic bands obtained from DFT and spectral function from DMFT.** Momentum-resolved spectral function  $A_{\mathbf{k}}(\epsilon)$  of CeH<sub>9</sub> along a high-symmetry path calculated with DMFT (color map) compared to the energy bands calculated by DFT (solid red lines).

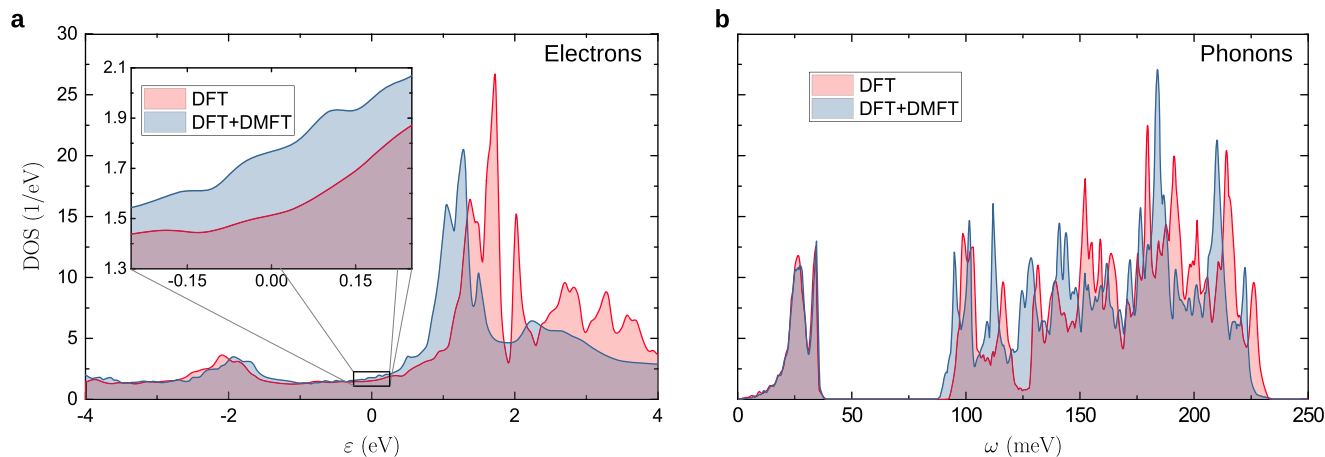
lines) to the DMFT spectral function (color map). As in LaH<sub>10</sub><sup>22</sup>, the dispersions around the Fermi level are dominated by H 1*s*-orbitals that hybridize considerably with the Ce 4*f*-orbitals, see Section S2 of the SI for additional details. Upon examining the intersections of the red bands and the high-intensity spectral features with the Fermi level (horizontal white line), we observe that the incorporation of electronic correlation effects results in a Fermi surface that remains largely unaltered in comparison to DFT calculations. In addition, the multiple electron and hole pockets remain qualitatively similar throughout the Brillouin zone. Quantitatively, however, higher-energy states are notably renormalized towards the Fermi level. For example, the electron pocket at the  $\Gamma$  point becomes 0.4 eV shallower as compared to the DFT result. Notable are the energy shifts of the non-dispersive Ce 4*f*-orbital bands, originally 1 to 2 eV above the Fermi level, which decrease significantly in DFT + DMFT computations.

By comparing the DFT+DMFT density of state (DOS) with the DFT one in Fig. 2a, we see that the inclusion of electronic correlations shifts the prominent Ce 4*f*-dominated spectral features down by at least 0.5 eV. Since the 4*f*-states are localized, their lowering causes the total spectral weight at the Fermi level to increase by 26%, as can be seen in the inset of Fig. 2a.

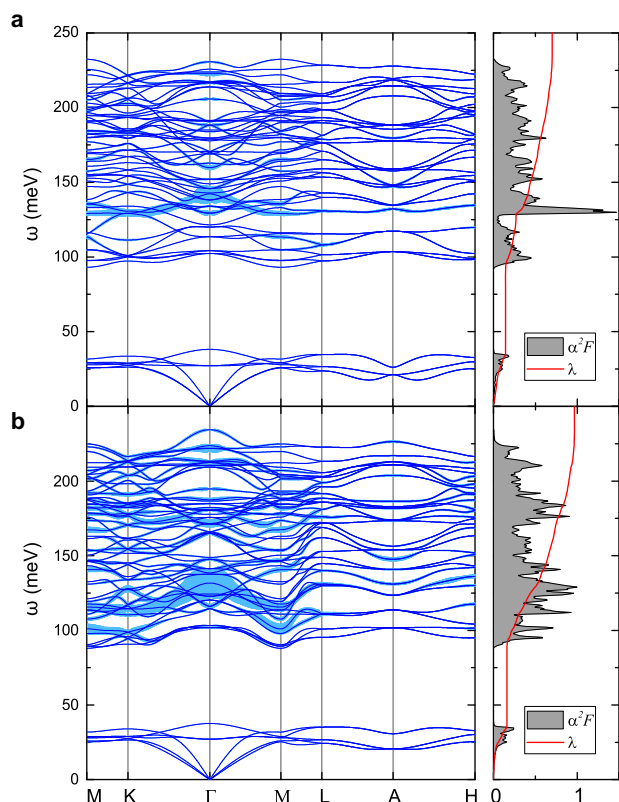
We also find that DFT+U, using the fully-localized-limit double-counting scheme, produces a DOS similar to DFT, see Fig. S5 of SI, suggesting that dynamical correlations drive the observed spectral changes. However, differences in the double-counting scheme between DFT+U and DFT+DMFT may also play a role. Meanwhile, the orbital occupation of Ce 4*f* increases slightly from 1.42 in DFT to 1.58 with DFT+DMFT. This charge transfer results in effective hole-doping of the H 1*s*-spectral weight. Wang et al.<sup>47</sup> noted that chemical hole doping can shift the electron pocket at  $\Gamma$  toward the Fermi level, enhancing the electron-phonon coupling. Remarkably, electronic correlations cause a similar effect in the stoichiometric compound. However, despite broadenings in DFT+DMFT, the excitation spectrum remains coherent and band-like. This can be understood by examining the local DFT+DMFT self-energy  $\Sigma_L(\epsilon)$ , from which we derive an averaged local quasiparticle weight  $Z = \frac{1}{N_L} \sum_L [1 - \frac{\partial \text{Re} \Sigma_L(\epsilon)}{\partial \epsilon} |_{\epsilon=\epsilon_F}]^{-1} = 0.8$ , where  $L$  is the 4*f* manifold with  $N_L = 7$ . The imaginary part of the self-energy is negligible around  $\pm 3$  eV of the Fermi level, allowing a quasiparticle description of the low-energy spectrum. See the Method Section and SI Section S3 for more details.

### Phonons in the presence of correlated electrons

We now investigate the impact of electronic correlations on the phonon modes. We compute phonon dispersion via the finite difference method<sup>49,50</sup>, at the DFT level using the forces arising from small atomic displacements and at the DFT+DMFT level using forces which are instead defined from the derivatives of the free energy  $F = E - TS$ , where  $T$  is the electronic temperature and  $S$  is the impurity entropy<sup>32</sup>. These calculations are enabled



**Fig. 2 | Comparison of density of states (DOS) per unit cell obtained from DFT and DMFT.** a Electronic and (b) phononic DOS of CeH<sub>9</sub> calculated with DFT and DFT+DMFT, respectively. The inset in (a) highlights the increase in the DOS near the Fermi level.



**Fig. 3 | Phonon and electron-phonon properties obtained from DFT and DMFT.** Phonon dispersion, Eliashberg spectral function  $\alpha^2F(\omega)$ , and integrated electron-phonon coupling strength  $\lambda(\omega)$  as a function of phonon frequency  $\omega$  as calculated with (a) DFT and (b) DFT+DMFT. The linewidth of the phonon dispersion is proportional to  $\lambda(\omega)$  projected onto the phonon modes.

by the efficient methodology from ref. 51. Figure 2 compares the phonon DOS of CeH<sub>9</sub> obtained within DFT and DFT+DMFT. Because of the significant difference in the atomic masses, the vibrations of cerium and hydrogen are largely decoupled, resulting in a clear energy separation in the phonon DOS. The low-frequency modes ( $\omega < 50$  meV) arise predominantly from cerium vibrations, while the high-frequency modes ( $\omega > 50$  meV) emerge from dynamical distortions of the hydrogen cages. The highest frequency reaches 240 meV at the DFT level (red curve), slightly lower than in LaH<sub>10</sub> in which the hardest mode reaches approximately 275 meV under similar pressure conditions<sup>52</sup>. The effect of DMFT is to soften hydrogen vibrations.

Given that the same structure is used in both approaches, we exclude a phonon softening through volume expansion and attribute it to electronic correlations captured by DMFT. This can be explained by the more localized nature of DMFT electrons, which have weaker chemical bonds, and is also observed in the iron-based superconductor with inelastic neutron scattering<sup>53</sup>.

### Superconductivity

Finally, we examine the influence of electronic correlations on the superconductivity of CeH<sub>9</sub>. To contextualize our results, it is worth first clarifying the hierarchy of methods used to evaluate the superconducting transition temperature ( $T_c$ ): (i) the McMillan-Allen-Dynes (AD) formula ( $T_c^{\text{AD}}$ )<sup>54,55</sup>, which provides a closed-form expression for  $T_c$  as follows

$$T_c^{\text{AD}} = \frac{\omega_{\text{ln}}}{1.2k_B} \exp \left[ \frac{-1.04(1 + \lambda)}{\lambda - \mu_c(1 + 0.62\lambda)} \right], \quad (1)$$

where  $\omega_{\text{ln}}$  is the logarithmic averaged phonon frequency,  $k_B$  denotes the Boltzmann constant,  $\lambda$  is the electron-phonon (el-ph) coupling strength,

and  $\mu_c$  is the Morel-Anderson pseudopotential accounting for Coulomb repulsion of the system<sup>56</sup>; (ii) the isotropic ( $T_c^{\text{iso}}$ ) and (iii) anisotropic Eliashberg equations ( $T_c^{\text{aniso}}$ )<sup>57,58</sup>, in which  $T_c$  is determined by identifying the highest temperature at which a nonzero superconducting gap  $\Delta$  appears. These three methods provide a progressively more refined description of phonon-mediated superconductivity with increasing accuracy and computational cost.

We note that Plekhanov et al.<sup>59</sup> have used the AD formula to obtain a correlation-induced enhancement in  $T_c$  with the many-body correction introduced directly at the level of the Eliashberg spectral function  $\alpha^2F(\omega)$ . They obtain a  $T_c^{\text{AD}} = 150$  K at 200 GPa, which overestimates the experimental value of 95 K<sup>9</sup>. This overestimation may be attributed to the use of the atomic Hubbard-I<sup>60</sup> solver for the DMFT impurity model and the use of DFT phonons. Our approach overcomes these limitations through the use of the continuous-time quantum Monte Carlo solver<sup>37,61</sup> which is unbiased towards electron localization, and by ensuring an equal-footing treatment of DMFT electrons and phonons.

Interestingly, with both electrons and phonons described at the DFT level, we find that the el-ph coupling strength for CeH<sub>9</sub> is  $\lambda = 2 \int_0^\infty d\omega \alpha^2F(\omega)/\omega = 0.70$ . We then compute the superconducting critical temperatures from the AD formula finding  $T_c^{\text{AD}} = 30$  K, and by solving the isotropic and anisotropic Eliashberg equations, leading to  $T_c^{\text{iso}} = 37$  K and  $T_c^{\text{aniso}} = 47$  K, respectively. As anticipated, the McMillan-Allen-Dynes estimate is the lowest, since that formula is formally valid only for low- $T_c$  superconductors. Our values for  $\lambda$ ,  $T_c^{\text{AD}}$  and  $T_c^{\text{iso}}$  agree well with a previous study<sup>9</sup>. The Eliashberg treatment improves the prediction. Importantly, the anisotropic Eliashberg solution demonstrates that anisotropy significantly increases the predicted  $T_c$ , bringing it closer to experimental observations.

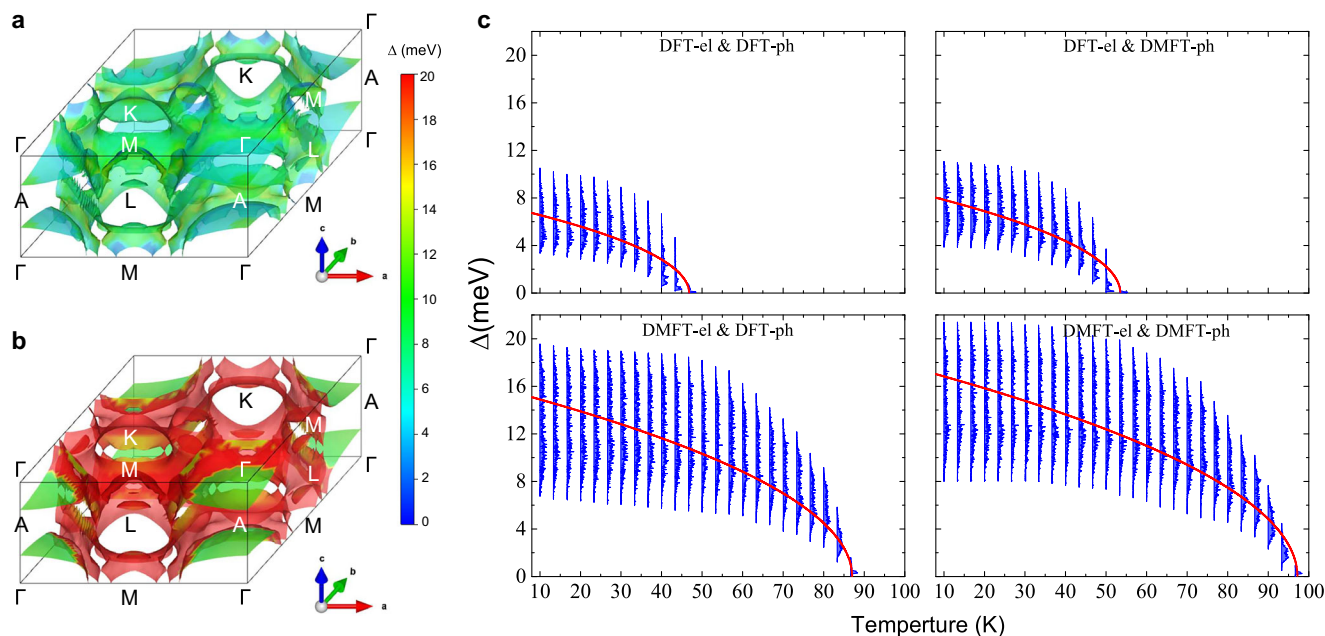
Figure 3a shows the integrated el-ph coupling strength  $\lambda(\omega) = 2 \int_0^\omega d\omega' \alpha^2F(\omega')/\omega'$ , el-ph coupling strength projected onto the phonon dispersion,  $\lambda_{\text{qv}}$ , and the Eliashberg function  $\alpha^2F(\omega)$ . We find that  $\lambda_{\text{qv}}$  is distributed in a nonuniform manner among the phonon modes and the phonon Brillouin zone, with approximately 80% of the total el-ph coupling strength arising from the optical phonon modes of hydrogen and the remaining 20% from the phonon modes of cerium. In particular, as highlighted by the linewidth in Fig. 3a, phonon modes with frequency around 125 meV are highly coupled to electrons, leading to a significant peak in the Eliashberg function  $\alpha^2F(\omega)$ . This frequency range is also where we observed a significant softening of the hydrogen mode by electronic correlations.

To go further, we substitute the electron Hamiltonian and phonon dynamical matrices obtained at the DFT level with their counterparts at the DMFT level. These two substitutions affect the electronic dispersion, the phonon dispersion, and the el-ph coupling matrix elements. We update the latter via the DMFT phonon eigendispersion and frequencies but we neglect the effect of DMFT on the perturbed electronic potential. Current implementations of the Migdal-Eliashberg theory of superconductivity are based on the quasiparticle approximation. Therefore, we construct from our DFT+DMFT calculations an effective quasiparticle band structure for CeH<sub>9</sub>. The construction of a renormalized band-structure is possible as the real-part of the self-energy can, to good approximation, be linearized around the Fermi level where its imaginary part is small. Then, an effective band structure can be found by upfolding the local DMFT self-energy into the Kohn-Sham basis  $\Sigma_{mn'k}(\epsilon) = \sum_L P_{mn'Lk} \Sigma_L(\epsilon)$  where  $P_{mn'Lk}$  is the inverse of the projector that defines the local  $4f$  basis<sup>31</sup>. In the DFT+DMFT, the charge density is obtained self-consistently, leading to an updated diagonal Kohn-Sham Hamiltonian  $H_{mnk}^{\text{DFT+DMFT}}$ . We obtain the renormalized quasiparticle energies  $E_{nk}$  by solving the following linearized equation<sup>62</sup>:

$$\det \left( E_{nk} \delta_{nn'} - \sum_m Z_{nmk} [H_{mn'k}^{\text{DFT+DMFT}} + \Re \Sigma_{mn'k}(\epsilon^F)] \right) = 0, \quad (2)$$

where

$$Z_{mn'k} = \left[ \delta_{mn'} - \frac{\partial \Re \Sigma_{mn'k}(\epsilon)}{\partial \epsilon} \Big|_{\epsilon=\epsilon^F} \right]^{-1} \quad (3)$$



**Fig. 4 | Anisotropic superconducting gap of CeH<sub>9</sub>.** Calculated superconducting gap  $\Delta$  on the Fermi surface at 10 K computed with (a) DFT and (b) DFT+DMFT. c Anisotropic Migdal-Eliashberg superconducting gap  $\Delta$  as a function of temperature. We consider four cases: (top left) DFT electrons with DFT phonons, (bottom left) DMFT electrons with DFT phonons, (top right) DFT electrons with DMFT

phonons, and (bottom right) DMFT electrons with DMFT phonons. The solid red line represents the temperature dependence of the superconducting gap expected from the BCS theory<sup>63</sup> in the weak-coupling limit where  $\Delta(T) = A\sqrt{1 - T/T_c}$ , where  $A$  is a fitting constant.

**Table 1 | Critical temperatures and superconducting parameters for CeH<sub>9</sub>**

|                                          | $T_c^{\text{aniso}}$<br>(K) | $T_c^{\text{iso}}$<br>(K) | $T_c^{\text{AD}}$<br>(K) | $P$<br>(GPa) | $\lambda$ | $\omega_{\text{in}}$<br>(meV) |
|------------------------------------------|-----------------------------|---------------------------|--------------------------|--------------|-----------|-------------------------------|
| This work                                |                             |                           |                          |              |           |                               |
| el <sup>DFT</sup> + ph <sup>DFT</sup>    | 47                          | 37                        | 30                       | 200          | 0.70      | 96                            |
| el <sup>DFT</sup> + ph <sup>DMFT</sup>   | 53                          | 43                        | 35                       | 200          | 0.71      | 108                           |
| el <sup>DMFT</sup> + ph <sup>DFT</sup>   | 87                          | 77                        | 59                       | 200          | 0.95      | 93                            |
| el <sup>DMFT</sup> + ph <sup>DMFT</sup>  | 96                          | 86                        | 69                       | 200          | 0.97      | 106                           |
| Prior works                              |                             |                           |                          |              |           |                               |
| el <sup>DFT</sup> + ph <sup>DFT12</sup>  | –                           | 50                        | –                        | 100          | 0.9       | –                             |
| el <sup>DFT</sup> + ph <sup>DFT47</sup>  | –                           | 74                        | –                        | 100          | 1.04      | –                             |
| el <sup>DFT</sup> + ph <sup>DFT9</sup>   | –                           | 49                        | 42                       | 150          | 0.85      | 93                            |
| el <sup>DFT</sup> + ph <sup>DFT9</sup>   | –                           | 31                        | 26                       | 200          | 0.68      | 109                           |
| el <sup>DFT</sup> + ph <sup>DFT13</sup>  | –                           | –                         | 74                       | 250          | 0.97      | 112                           |
| el <sup>DMFT</sup> + ph <sup>DFT59</sup> | –                           | –                         | 150                      | 200          | 1.06      | 154                           |
| experiment <sup>9</sup>                  | 95                          | –                         | –                        | 110          | –         | –                             |
| experiment <sup>9</sup>                  | 95                          | –                         | –                        | 150          | –         | –                             |
| experiment <sup>10</sup>                 | 110                         | –                         | –                        | 110          | –         | –                             |
| experiment <sup>11</sup>                 | 90                          | –                         | –                        | 116          | –         | –                             |

We report the logarithmic averaged phonon frequency ( $\omega_{\text{in}}$ ) and electron-phonon coupling strength ( $\lambda$ ) entering the Allen-Dyne  $T_c^{\text{AD}}$ , isotropic Migdal-Eliashberg  $T_c^{\text{iso}}$ , and anisotropic Migdal-Eliashberg  $T_c^{\text{aniso}}$ . Our calculations describe the electron-phonon pairing on four levels of sophistication and are compared to previous theoretical works at the DFT level and experimental measurements. All theoretical values of  $T_c$  reported in the table are calculated with the Morel-Anderson pseudopotential  $\mu_c = 0.13$  except ref. 9 which uses  $\mu_c = 0.15$ .

is the quasiparticle weight which approaches unity in a noninteracting system and zero in the limit of extremely strong correlations.

We validate the quality of the effective band-structure obtained using the above quasiparticle approximation in Section S4 of the SI. Using this

effective band structure and the DMFT phonon spectrum obtained previously, we calculate the el-ph coupling strength and the Eliashberg function at the DMFT level, as shown in Fig. 3b. The total coupling strength in this case is found to increase by nearly 39%, reaching  $\lambda = 0.97$ . This increase supports a substantial elevation in the critical temperature, which increases from  $T_c^{\text{AD}} = 30$  K at the DFT level to  $T_c^{\text{AD}} = 69$  K at the DMFT level. We traced the increase in  $T_c$  to changes in specific regions in the Brillouin zone.

Figure 4a, b compare the superconducting gap  $\Delta$  on the Fermi surface of CeH<sub>9</sub> at 10 K. We find that in the case of DFT the superconducting gap is quite uniform across the Fermi surface, with an average magnitude of approximately 6.3 meV that varies by  $\pm 2.5$  meV through the Brillouin zone. In contrast, at the DMFT level, the superconducting gap around the corner of the Brillouin zone (i.e. the  $K$  point) exhibits a remarkable increase, up to 20 meV, which explains the elevated superconducting critical temperature, from  $T_c^{\text{aniso}} = 47$  K at the DFT level to  $T_c^{\text{aniso}} = 96$  K at the DMFT level.

To gain further insights into the role of electronic correlation, we consider two ‘intermediate scenarios’ of el-ph coupling: DMFT electrons are paired with DFT phonons, and DFT electrons are paired with DMFT phonons. Figure 4c shows the energy distribution of the superconducting gap  $\Delta$  as a function of temperature for our previous results at the DFT and DMFT levels, as well as for the two intermediate scenarios. The superconducting gap is seen to close gradually with increasing temperature, vanishing at various critical values for each case. Table 1 summarizes the critical temperatures obtained, together with the corresponding superconducting parameters, offering a hierarchical comparison also with existing DFT studies and experimental measurements.

Our results align closely with previous DFT studies but overestimate experimental values at comparable pressures by 50%. In contrast, our value at the DMFT level,  $T_c^{\text{aniso}} = 96$  K at 200 GPa, is in excellent agreement with the experimental value,  $T_c = 95$  K at the closest pressure of 150 GPa. Dissecting the influence of electronic correlations on the different ingredients entering the calculation of  $T_c$ , we find that the DMFT renormalization of the electronic structure is the main driving force behind the increased critical temperature. Indeed, keeping the phonons at the DFT level, the effect of DMFT on electrons almost doubles the  $T_c$ . Indeed, as shown in Fig. 2a, the

increased DOS at the Fermi level,  $D(\epsilon_F)$ , facilitates the formation of more Cooper pairs, leading to a higher superconducting critical temperature for which  $T_c \propto \exp(-\frac{1}{VD(\epsilon_F)})$  where  $V$  is the pairing interaction<sup>63</sup>. Finally, we also discover that exclusively renormalizing the electronic structure with DMFT still leads to a substantial underestimation of the superconducting critical temperature. It is necessary to also include the phonon-softening effect due to electronic correlations to quantitatively reconcile the theoretical findings with experimental data.

## Discussion

In summary, we have used a combination of DFT and DMFT to study electrons and phonons of CeH<sub>9</sub> under high pressure, demonstrating that strong electronic correlations arising from cerium  $4f$ -states play an important role in this system. Many-body effects increase electron masses, produce a larger spectrum at the Fermi level, and soften hydrogen vibrational modes. Combining DFT+DMFT with the Migdal-Eliashberg theory of superconductivity, we were able to investigate the role of electronic correlations for the critical temperatures of phonon-mediated superconductivity in CeH<sub>9</sub>. Our findings indicate that the dominant correction to the critical temperature comes from the many-body renormalization of the electronic structure. However, we find that the renormalization of phonons is significant and cannot be neglected. The many-body-driven increase in the critical superconducting temperature is 50 K. Future extensions of this work should address the impact of many-body correlations on the perturbed potential, given that exchange and correlation effects beyond semi-local DFT can either increase<sup>64–68</sup> or decrease<sup>69,70</sup> the values of the el-ph coupling matrix elements.

Overall, the renormalized Migdal-Eliashberg approach developed here is not specific to CeH<sub>9</sub> but can be applied to other compounds where el-ph interactions coexist with electronic correlations. Promising targets include transition-metal hydrides with partially filled  $d$ -shells, such as X<sub>2</sub>MH<sub>6</sub> (where X are alkali, alkaline-earth, or post-transition metals and M are  $3d$ -,  $4d$ -, and  $5d$ -transition metals) which have recently attracted attention for their potential high-temperature superconductivity at ambient pressure<sup>71</sup>. In addition, while our approach focuses on phonon-mediated superconductivity, it could serve as a reference point to assess the relative importance of el-ph coupling effects in materials where other mechanisms such as spin-fluctuations<sup>72,73</sup> dominate. Future developments incorporating electronic self-energy effects beyond the Migdal-Eliashberg theory may help clarify how phonons influence unconventional superconductivity in these systems.

## Methods

### Electronic structure calculations

We have performed DFT+DMFT calculations at inverse temperature  $\beta = 20 \text{ eV}^{-1}$  (i.e.  $T \simeq 580 \text{ K}$ ) with the embedded DMFT functional package EDMFT<sup>32</sup> integrated with the all-electron DFT code WIEN2K<sup>74</sup> for both electrons and phonons in CeH<sub>9</sub>. A single calculation at a lower temperature with  $\beta = 100 \text{ eV}^{-1}$  (i.e.  $T \simeq 116 \text{ K}$ ) has also been performed to examine possible effects of temperature onto the electronic self-energy. The resulting self-energy was found to fall on top of that obtained at  $\beta = 20 \text{ eV}^{-1}$  (see Fig. S6a). The DMFT impurity problem is solved using a continuous-time quantum Monte Carlo algorithm<sup>37,61</sup>. We use the nominal double-counting scheme<sup>37</sup>, with an occupation fixed to 2, as the DFT-calculated valency of Ce under pressure is found to be 1.42 (greater than the nominal 1 electron) indicating an increased  $f$ -electron occupancy compared to the idealized trivalent state. The impact of the choice of the nominal occupation values on the self-energy has been examined in Section S5 of the SI, where the quasiparticle renormalization factor is found to be independent when the nominal occupation varies from 1 to 2. The corresponding DMFT occupation is increasing from 1.11 to 1.58 for the same range. The standard nominal occupation for (unpressurized) Ce-compounds,  $n_f^0 = 1$ , corresponds to a Ce<sup>3+</sup> configuration for pressurized CeH<sub>9</sub>, which we find implausible given the DFT valency for CeH<sub>9</sub>. We also note that the magnetic susceptibility of CeH<sub>9</sub> exhibits no long-term memory, see SI Section S6, indicating the absence of fluctuating local moments in CeH<sub>9</sub>. Details of Haule et al.'s implementation can be found in ref. 32. We analytically

continue the Matsubara self-energy to real frequencies using the maximum entropy method<sup>75</sup>. The quasiparticle weight was extracted from both Matsubara and real-frequency data and was found to be consistent. We have cross-checked the WIEN2K all-electron results with the pseudopotential-based DFT packages CASTEP<sup>76,77</sup> and QUANTUM ESPRESSO<sup>78,79</sup> that were used previously in ref. 59, using the same ultrasoft pseudopotentials that CASTEP generates on the fly for both codes. The valence electron configurations of  $5s^2 5p^6 4f^5 5d^1 6s^2$  (with  $4f$ -electrons explicitly included) and  $1s$  are adopted for the Ce and H atoms, respectively. Figure S11 in SI Section S7 shows close agreement between the three codes. Convergence tests at the DFT level yielded an energy cut-off of 800 eV for CASTEP and for QUANTUM ESPRESSO. For WIEN2K, convergence is achieved when the product of the smallest atomic-sphere radius and the maximum reciprocal-space vector in the plane-wave expansion reaches 7. A  $\Gamma$ -centered  $\mathbf{k}$ -point grid of size  $12 \times 12 \times 6$  is used for all three packages.

The exchange-correlation functional is approximated using PBE<sup>80</sup>. As was done in previous works<sup>9,12,13,47,59</sup>, we omit spin-orbit coupling for technical reasons. In the DFT + DMFT calculations, we use an on-site Coulomb interaction (Hubbard  $U$ ) of  $U = 6.0 \text{ eV}$  and a Hund's coupling  $J = 0.7 \text{ eV}$  for the cerium  $f$  orbitals. This choice is comparable to previous values that were successfully used for elemental cerium<sup>35–38</sup>, CeH<sub>9</sub><sup>59</sup>, and other Ce-compounds<sup>44</sup>. Note that we neglect any potential impact of pressure on Hubbard  $U$ <sup>41,81</sup>. We also omit any additional renormalizations of the DMFT electronic structure that arise from the electron-phonon coupling<sup>82,83</sup>.

### Lattice dynamics calculations

For the lattice dynamics calculations, we use finite difference with an in-house code which offers a versatile interface with DFT and DFT+DMFT<sup>51</sup>, to calculate the phonon spectrum of CeH<sub>9</sub>. Considering that the computational cost of DFT+DMFT exhibits a particularly unfavorable scaling with the system size, we employ the non-diagonal supercell technique<sup>84</sup> to sample a  $2 \times 2 \times 2$   $\mathbf{q}$ -point grid in the Brillouin zone and then interpolate the result to obtain dynamical matrices on a  $\mathbf{q}$ -point grid of  $6 \times 6 \times 3$ . A convergence validation of the phonon dispersions with the size of the  $\mathbf{q}$ -point grid at the DFT level is provided in Section S8 of the SI. In addition, we find that the fixed self-energy approximation<sup>51</sup> is not applicable to CeH<sub>9</sub>, see Sec. S9 of the SI, and thus fully self-consistent DFT+DMFT calculations are performed for each displaced configuration. Specifically, we use four different supercells constructed with the following supercell matrices:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \text{ and } \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 1 & 2 & 0 \end{pmatrix},$$

the first one provides access to the  $\Gamma$   $\mathbf{q}$ -point, then the second one provides access to the  $(0, 0, 1/2)$   $\mathbf{q}$ -point, the third one to the  $(0, 1/2, 0)$   $\mathbf{q}$ -point, and the fourth one to the  $(1/2, 1/2, 1/2)$   $\mathbf{q}$ -point. All other  $\mathbf{q}$ -points on the  $2 \times 2 \times 2$  grid are related to these four by symmetry and therefore explicit calculations are not necessary.

### Superconductivity calculations

To evaluate the superconducting critical temperature  $T_c$ , we used EPW<sup>85,86</sup> to interpolate the el-ph coupling matrix calculated with the density functional perturbation theory as implemented in QUANTUM ESPRESSO from a  $12 \times 12 \times 6$   $\mathbf{k}$ -point grid and a  $6 \times 6 \times 3$   $\mathbf{q}$ -point grid to a  $48 \times 48 \times 24$   $\mathbf{k}$ -point grid and a  $24 \times 24 \times 12$   $\mathbf{q}$ -point grid. In particular, for  $T_c$  calculations at the DFT+DMFT level, the electronic and phononic degrees of freedom obtained from standard DFT are replaced with the counterparts obtained from DFT+DMFT. We used a standard value for the Morel-Anderson pseudopotential  $\mu_c = 0.13$  which accounts for Coulomb repulsion of the system<sup>56</sup> in all our calculations.

### Data availability

The data and codes that support the findings of this study are available in the Supplementary Information and on the Materials Cloud Archive at <https://>

doi.org/10.24435/materialscloud:hw-nk. The WIEN2K v21.1 code used in this study is a commercial software, available from <http://susi.theochem.tuwien.ac.at>. The QUANTUM ESPRESSO v7.0 code used in this research is open source: <https://www.quantum-espresso.org>. The CASTEP 23.1 code used in this study is freely available at <https://www.castep.org> for academic research. The EPW v5.4.1 code used in this research is open source: <https://epw-code.org>. The ANA\_CONT v1.1.2 code used in this study is open source: [https://github.com/josefkaufmann/ana\\_cont](https://github.com/josefkaufmann/ana_cont). Haule et al. provide their DMFT package (Oct-2024 release) at <https://github.com/ru-cmmt/eDMFT>.

## Code availability

The WIEN2K v21.1 code used in this study is a commercial software, available from <http://susi.theochem.tuwien.ac.at>. The QUANTUM ESPRESSO v7.0 code used in this research is open source: <https://www.quantum-espresso.org>. The CASTEP 23.1 code used in this study is freely available at <https://www.castep.org> for academic research. The EPW v5.4.1 code used in this research is open source: <https://epw-code.org>. The ANA\_CONT v1.1.2 code used in this study is open source: [https://github.com/josefkaufmann/ana\\_cont](https://github.com/josefkaufmann/ana_cont). Haule et al. provide their DMFT package (Oct-2024 release) at <https://github.com/ru-cmmt/eDMFT>.

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### Author contributions

S.C. and Y.W. contributed equally to this work. S.C. performed the DMFT spectral function and superconducting calculations, while Y.W. performed the DMFT phonon calculations. S.P. and J.M.T provided technical help with the WIEN2K and EPW software. S.P., B.M. and J.M.T supervised the work. All authors reviewed and approved the final version of the manuscript.

### Competing interests

The authors declare no competing interests.

### Additional information

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