Supplementary Information: Exact double-counting in combining the Dynamical Mean Field Theory and the Density Functional Theory

THE CORRELATION ENERGY FIT

The correlation energy of the electron gas, interacting with Yukawa potential, was calculated by G_0W_0 method, and fitted with the following functional form

$$\varepsilon^c_{V^\lambda_c} = \frac{\varepsilon^c_{\lambda=0}}{1 + \sum_{n=1}^{4} a_n r_s^n} \tag{1}$$

Here $\varepsilon^c_{\lambda=0}$ is the standard parametrization of the correlation energy of the electron gas.

For the coefficients a_n, we chose the following form:

$$\log(1 + a_1) = \frac{\lambda(\alpha_0 + \alpha_1\lambda)}{1 + \alpha_2\lambda^2 + \alpha^3\lambda^4 + \alpha_4\lambda^6} \tag{2}$$

$$\log(1 + a_2) = \frac{\lambda^2(\beta_0 + \beta_1\lambda)}{1 + \beta_2\lambda^2 + \beta_3\lambda^4} \tag{3}$$

$$\log(1 + a_3) = \frac{\lambda^3(\gamma_0 + \gamma_1\lambda)}{1 + \gamma_2\lambda^2} \tag{4}$$

$$\log(1 + a_4) = \lambda^4(\delta_0 + \delta_1\lambda^2) \tag{5}$$

The best fit, in the range $r_s \in [0, 10]$ and $\lambda \in [0, 3]$, gives the following coefficients:

$$\begin{aligned}
\alpha_i &= [1.2238912, 7.3648662, 9.6044695, \\
&\qquad -0.7501634, 0.0207808] \times 10^{-1} \\
\beta_i &= [5.839362, 11.969474, 10.156124, 1.594125] \times 10^{-2} \\
\gamma_i &= [8.27519, 5.57133, 17.25079] \times 10^{-3} \\
\delta_i &= [5.29134419, 0.0449628225] \times 10^{-4}
\end{aligned} \tag{6}$$

NOTE ON DERIVATION OF THE EXACT DOUBLE-COUNTING

Most of the double-counting formulas were historically derived by approximating the Hubbard interaction term (defined with the help of matrix elements Eq. 33) by some static approximation, either in the atomic limit, or, in Hartree-Fock limit. Such static approximations were argued to be a good substitute for the LDA treatment of the Hubbard interaction. Hence, the problem arrose, because it is not clear how to solve the Hubbard model (or any lattice model) by LDA, so that the LDA approximation for the Hubbard term could be subtracted from dynamic self-energy, computed by many body method.

Here we show that, if Luttinger-Ward functionals for the two approximate methods are written side-by side in the same form, the intersection of the two is evident. In other words, we can either perform the DMFT approximation on the LDA functional, or, the LDA approximation on the DMFT functional, and in both cases we arrive at the same term, which is counted twice.

Let's start with the lowest order term in the interaction, the Hartree term, because it can be explicitly written down. The exact Hartree term takes the form

$$E^H[\rho] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \tag{7}$$

In the DMFT approximation, the Hartree term is approximated by its local and screened counterpart:

$$E^H_{DMFT}[\rho] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' (\hat{P}\rho(\mathbf{r}))(\hat{P}\rho(\mathbf{r}')) V_{DMFT}(|\mathbf{r} - \mathbf{r}'|) \tag{8}$$

Notice that when this expression is written in orbital basis, it gives exactly the Hartree term, which appears in DMFT.

The LDA implementation includes the exact Hartree term Eq. 7, and the DMFT includes the approximation Eq. 8. When the two Luttinger-Ward functionals are added in LDA+DMFT, we must subtract the entire DMFT approximation for Hartree term Eq. 8, because this term was already accounted for by LDA exactly, hence no extra DMFT term is needed to this order.

Next we consider the exchange term. The exact exchange takes the following form:

$$E^X[\rho] = -\frac{1}{2} \sum_\sigma \int d\mathbf{r} d\mathbf{r}' \frac{\rho_\sigma(\mathbf{r}, \mathbf{r}')\rho_\sigma(\mathbf{r}', \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \tag{9}$$

However, the LDA method does not take into account the exact exchange term, but it approximates it with the following approximation

$$E^X_{LDA} = -\frac{1}{2} \sum_\sigma \int d\mathbf{r} d\mathbf{r}' \rho^0_\sigma(\mathbf{r}, \mathbf{r}')\rho^0_\sigma(\mathbf{r}', \mathbf{r})V_c(|\mathbf{r} - \mathbf{r}'|) \tag{10}$$

where ρ^0 is the charge density of the corresponding electron gas problem, namely,

$$\rho^0_\sigma(\mathbf{r}, \mathbf{r}') = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')} f(\frac{k^2}{2m} - E_F) \tag{11}$$

where f is the fermi function (at $T = 0$) and $E_F = (2\pi^2\rho)^{2/3}/(2m)$.

Notice that the LDA exchange is obtained from Eq. 9 by replacing the density $\rho_\sigma(\mathbf{r}, \mathbf{r}')$ of the solid by the simpler density of the electron gas problem, ρ^0_σ. The only place where the real solid and electron gas problem are linked, is through the determination of the charge density, or equivalent, the determination of E_F of the corresponding electron gas problem.

The DMFT approximates the exact exchange Eq. 9 by the following truncation of variables,

$$\rho \to \hat{P}\rho \tag{12}$$
$$V_c \to V_{DMFT} \tag{13}$$

hence the DMFT includes the following exchange term

$$E^X_{DMFT} = -\frac{1}{2} \sum_\sigma \int d\mathbf{r} d\mathbf{r}' (\hat{P}\rho_\sigma(\mathbf{r}, \mathbf{r}'))(\hat{P}\rho_\sigma(\mathbf{r}', \mathbf{r}))V_{DMFT}(|\mathbf{r} - \mathbf{r}'|) \tag{14}$$

To prove that, we recall the definition of the projector $\hat{P}$ (defined in Eq. 30)

$$\hat{P}\rho(\mathbf{r}, \mathbf{r}') = \sum_{L_1, L_2 \in DMFT} \langle\mathbf{r}|\Phi_{L_1}\rangle \langle\Phi_{L_1}|\rho(\mathbf{r}, \mathbf{r}')|\Phi_{L_2}\rangle \langle\Phi_{L_2}|\mathbf{r}'\rangle \tag{15}$$

where $L_1, L_2 \in DMFT$ denotes the sum over the orbitals treated by DMFT. Inserting this definition into the above Eq. 14, it is immediately evident that

$$E^X_{DMFT} = -\frac{1}{2} \sum_{\{L_i\} \in DMFT} \int d\mathbf{r} d\mathbf{r}' \Phi_{L_4}(\mathbf{r}) \langle\Phi_{L_4}|\rho|\Phi_{L_2}\rangle \Phi^*_{L_2}(\mathbf{r}')\Phi_{L_3}(\mathbf{r}') \langle\Phi_{L_3}|\rho|\Phi_{L_1}\rangle \Phi^*_{L_1}(\mathbf{r})V_{DMFT}(|\mathbf{r} - \mathbf{r}'|) \tag{16}$$

In the integral we recognize the matrix elements of the screened Coulomb interaction (used in DMFT):

$$U_{L_1, L_2, L_3, L_4} = \int d\mathbf{r} d\mathbf{r}' \Phi^*_{L_1}(\mathbf{r})\Phi^*_{L_2}(\mathbf{r}')V_{DMFT}(|\mathbf{r} - \mathbf{r}'|)\Phi_{L_3}(\mathbf{r}')\Phi_{L_4}(\mathbf{r}) \tag{17}$$

and the DMFT density matrix, which is

$$n_{L_1, L_2} = \frac{1}{\beta} \sum_{i\omega} \langle\Phi_{L_2}|G(i\omega, \mathbf{r}\mathbf{r}')|\Phi_{L_1}\rangle = \langle\Phi_{L_2}|\rho|\Phi_{L_1}\rangle \tag{18}$$
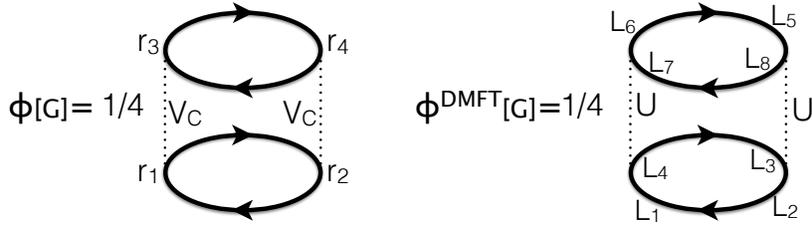
FIG. 1: The second order Feynman graph of the exact functional $\Phi[\{G\}]$ on the left, and the corresponding DMFT functional $\Phi^{DMFT}[\{G_{local}\}]$ on the right.

Using these standard definitions, we immediately recognize

$$E_{DMFT}^X = -\frac{1}{2}\sum_{\{L_i\}in DMFT} U_{L_1,L_2,L_3,L_4} n_{L_1,L_3} n_{L_2,L_4}, \tag{19}$$

which is the standard form for the DMFT exchange energy. This term is included when solving the DMFT quantum impurity problem.

Now, having both LDA and DMFT functionals for exchange written in the same form, Eq. 10 and Eq. 14, it becomes clear how to perform the LDA approximation on the DMFT functional, or, the DMFT approximation on the LDA functional. This is the double-counting term.

In the DMFT approximation on top of LDA functional Eq. 10, we need to replace V_c with V_{DMFT} and replace ρ in the electron gas fermi level EF with ρ_{local}. When performing LDA approximation on the DMFT functional Eq. 14, we replace real density $\hat{P}\rho$ by ρ^0 of electron gas, and determine the fermi level EF by the density of the solid $\hat{P}\rho = \rho_{local}$. In both cases, we arrive at the exact intersection of the two methods (for exchange term):

$$E_{DC}^X = -\frac{1}{2}\int d\mathbf{r} d\mathbf{r}' \rho_\sigma^0(\mathbf{r},\mathbf{r}')\rho_\sigma^0(\mathbf{r}',\mathbf{r}')V_{DMFT}(|\mathbf{r}-\mathbf{r}'|) \tag{20}$$

where

$$\rho^0(\mathbf{r},\mathbf{r}') = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f(\frac{k^2}{2m} - E_F) \tag{21}$$

and

$$E_F = (2\pi^2\hat{P}\rho)^{2/3}/(2m) = (2\pi^2\hat{P}\rho_{local})^{2/3}/(2m).$$

We can continue the same derivation for the correlation term.

First we prove one of the central assumptions in the manuscript, namely, that performing the DMFT approximation is equivalent to performing the following approximation on the exact $\Phi[G]$ functional: replacing $G(\mathbf{r},\mathbf{r}')$ by $\hat{P}G(\mathbf{r},\mathbf{r}') = G_{local}(\mathbf{r},\mathbf{r}')$ and V_c by V_{DMFT}. The form of the functional does not change.

We can show this order by order in perturbation theory. We already showed it for the first order terms, namely, the Hartree and the Fock term. We next show it also for the second order term, displayed in Fig. 1

The exact functional contribution at the second order is

$$\Phi[\{G\}] = \frac{1}{4}\int\prod_{i=1}^4 d\mathbf{r}_i \int_0^\beta d\tau V_c(\mathbf{r}_3-\mathbf{r}_1)V_c(\mathbf{r}_4-\mathbf{r}_2)G(\mathbf{r}_1,\mathbf{r}_2,\tau)G(\mathbf{r}_2,\mathbf{r}_1,-\tau)G(\mathbf{r}_4,\mathbf{r}_3,-\tau)G(\mathbf{r}_3,\mathbf{r}_4,\tau) \tag{22}$$

According to the above assumption, the corresponding DMFT contribution must take the form

$$\Phi^{DMFT}[\{G_{local}\}] = \frac{1}{4}\int\prod_{i=1}^4 d\mathbf{r}_i \int_0^\beta d\tau V_{DMFT}(\mathbf{r}_3-\mathbf{r}_1)V_{DMFT}(\mathbf{r}_4-\mathbf{r}_2)G_{local}(\mathbf{r}_1,\mathbf{r}_2,\tau)G_{local}(\mathbf{r}_2,\mathbf{r}_1,-\tau)G_{local}(\mathbf{r}_4,\mathbf{r}_3,-\tau)G_{local}(\mathbf{r}_3,\mathbf{r}_4,\tau)$$

$$\tag{23}$$

To prove that, we just insert definition for G_{local} (Eq. 30) into the above equation, and obtain

$$\Phi^{DMFT}[\{G_{local}\}] = \frac{1}{4} \int \prod_{i=1}^{4} d\mathbf{r}_i \int_0^\beta d\tau \sum_{\{L_i\}} V_{DMFT}(\mathbf{r}_3 - \mathbf{r}_1) V_{DMFT}(\mathbf{r}_4 - \mathbf{r}_2) \Phi_{L_1}(\mathbf{r}_1) \langle \Phi_{L_1}|G(\tau)|\Phi_{L_2}\rangle \Phi_{L_2}^*(\mathbf{r}_2)$$
$$\times \Phi_{L_3}(\mathbf{r}_2) \langle \Phi_{L_3}|G(-\tau)|\Phi_{L_4}\rangle \Phi_{L_4}^*(\mathbf{r}_1)$$
$$\times \Phi_{L_5}(\mathbf{r}_4) \langle \Phi_{L_5}|G(-\tau)|\Phi_{L_6}\rangle \Phi_{L_6}^*(\mathbf{r}_3)$$
$$\times \Phi_{L_7}(\mathbf{r}_3) \langle \Phi_{L_7}|G(\tau)|\Phi_{L_8}\rangle \Phi_{L_8}^*(\mathbf{r}_4) \quad (24)$$

which is equal to

$$\Phi^{DMFT}[\{G_{local}\}] = \frac{1}{4} \int_0^\beta d\tau \sum_{\{L_i\}} \int d\mathbf{r}_1 d\mathbf{r}_3 \Phi_{L_4}^*(\mathbf{r}_1)\Phi_{L_6}^*(\mathbf{r}_3) V_{DMFT}(\mathbf{r}_3 - \mathbf{r}_1) \Phi_{L_7}(\mathbf{r}_3)\Phi_{L_1}(\mathbf{r}_1)$$
$$\times \int d\mathbf{r}_2 d\mathbf{r}_4 \Phi_{L_2}^*(\mathbf{r}_2)\Phi_{L_8}^*(\mathbf{r}_4) V_{DMFT}(\mathbf{r}_4 - \mathbf{r}_2) \Phi_{L_5}(\mathbf{r}_4)\Phi_{L_3}(\mathbf{r}_2)$$
$$\times \langle \Phi_{L_1}|G(\tau)|\Phi_{L_2}\rangle \langle \Phi_{L_3}|G(-\tau)|\Phi_{L_4}\rangle$$
$$\times \langle \Phi_{L_5}|G(-\tau)|\Phi_{L_6}\rangle \langle \Phi_{L_7}|G(\tau)|\Phi_{L_8}\rangle \quad (25)$$

Using the definition of the screened Coulomb repulsion Eq. 17, and the definition for the DMFT Green's function, we obtain

$$\Phi^{DMFT}[\{G_{local}\}] = \frac{1}{4} \int_0^\beta d\tau \sum_{\{L_i\}} U_{L_4,L_6,L_7,L_1} U_{L_2,L_8,L_5,L_3} G_{L_1,L_2}^{local}(\tau) G_{L_3,L_4}^{local}(-\tau) G_{L_5,L_6}^{local}(-\tau) G_{L_7,L_8}^{local}(\tau), \quad (26)$$

which is just the Feynman diagram that appears in the DMFT impurity problem. It is clear from this derivation that we can do the same procedure for any Feynman diagram of any complex topology, hence, we can also perform the substitution directly in the functional. This proves the central assumption of the paper, namely, what is the DMFT approximation. This proof already appeared in Ref. [1], but for completness, we repeated it here.

On the other hand, the LDA approximation to the exact functional $\Phi[G]$ amounts to mapping the system, point by point in 3D space, to the electron gas problem

$$\Phi[\{G\}] \to E_{V_c}^C[\rho] = \int d\mathbf{r} E_{el-gas}^C(\rho(\mathbf{r}); V_c) \quad (27)$$

where $E_{el-gas}^C(\rho^0; V_c)$ is the correlation energy of the electron gas problem, interacting with the Coulomb interaction V_c, at the density ρ^0.

Finally, we perform the DMFT approximation on the LDA correlation functional, which amounts to replacing ρ by $\hat{P}\rho$ and V_c by V_{DMFT}, and we obtain

$$\Phi^{DC}[\{G\}] \to \int d\mathbf{r} E_{el-gas}^C(\hat{P}\rho(\mathbf{r}); V_{DMFT}), \quad (28)$$

hence we need to solve the electron gas problem at each point in space, where the charge $\hat{P}\rho$ interacts with screened interaction V_{DMFT}. We can symbolically write this term as $E_{V_{DMFT}}^C[\hat{P}\rho]$. In this derivation we performed DMFT approximation on the LDA functional. We could equally well perform the LDA approximation on the DMFT functional, and get the same result.

To summarize, the double-counting term, which we derived, takes the following form

$$\Phi_{DC}^{DFT+DMFT}[\rho] = E_{V_{DMFT}}^H[\hat{P}\rho] + E_{V_{DMFT}}^{XC}[\hat{P}\rho]. \quad (29)$$

THE DMFT PROJECTOR

The DMFT local Green's function is obtained from the total Green's function of the solid by a projection, defined by

$$G_{local}(\mathbf{r}, \mathbf{r}') = \sum_{L,L'} \langle \mathbf{r}|\phi_L\rangle \langle \phi_L| G |\phi_{L'}\rangle \langle \phi_{L'}|\mathbf{r}'\rangle \quad (30)$$
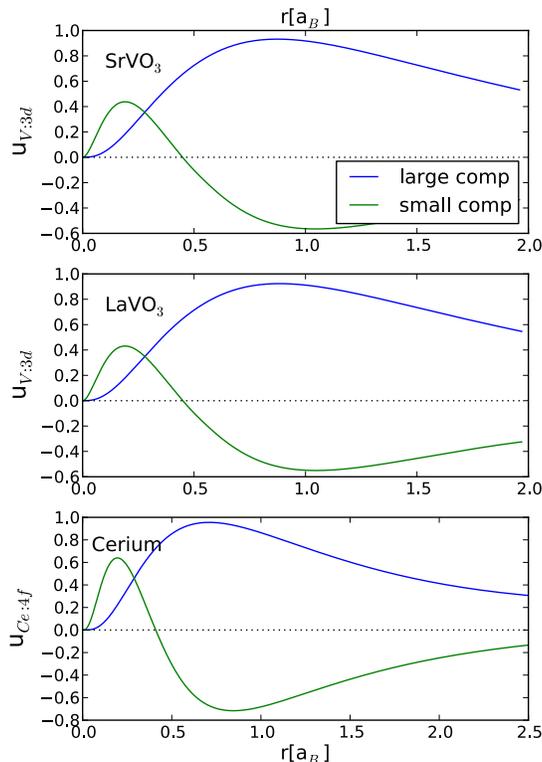
FIG. 2: The radial wave functions $u_l(r)$, which are used to build the DMFT projector and the local Green's function. We show both the large and the small component of the solution of the Dirac equation.

where the quasi-localized wave functions $\langle \mathbf{r} | \phi_L \rangle = \frac{u_l(r)}{r} Y_L(\mathbf{r})$ are the solution of the Dirac equation inside the muffin-tin sphere in the scalar relativistic approximation. The linearization energy E_ν is here chosen at the Fermi level $E_\nu = E_F$, to have very precise wave function in the vicinity of the Fermi level.

The extremization of the DMFT functional leads to the Dyson equation (Equation 2 of the main text), in which the embedding operator is usually needed [3]. In the real space representation of the DMFT, however, the embedding operator is replaced by the projection operator itself. To show this, we take the functional derivative of the DMFT term

$$\Sigma(\mathbf{r}', \mathbf{r}) = \frac{\delta \Phi[G_{local}]}{\delta G(\mathbf{r}, \mathbf{r}')} = \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\delta G_{local}(\mathbf{r}_1, \mathbf{r}_2)}{\delta G(\mathbf{r}, \mathbf{r}')} \frac{\delta \Phi[G_{local}]}{\delta G_{local}(\mathbf{r}_1, \mathbf{r}_2)} = \sum_{L,L'} \langle \mathbf{r}' | \phi_L \rangle \langle \phi_L | \frac{\delta \Phi[G_{local}]}{\delta G_{local}} | \phi_{L'} \rangle \langle \phi_{L'} | \mathbf{r} \rangle = \hat{P} \frac{\delta \Phi[G_{local}]}{\delta G_{local}} \quad (31)$$

hence $\Sigma = \hat{P} \frac{\delta \Phi[G_{local}]}{\delta G_{local}}$ instead of $\Sigma = \hat{E} \frac{\delta \Phi[G_{local}]}{\delta G_{local}}$, as is in the orbital/band representation. In this derivation we used the following identify

$$\frac{\delta G_{local}(\mathbf{r}_1, \mathbf{r}_2)}{\delta G(\mathbf{r}, \mathbf{r}')} = \sum_{L,L'} \phi_L(\mathbf{r}_1) \phi_L^*(\mathbf{r}) \phi_{L'}(\mathbf{r}') \phi_{L'}^*(\mathbf{r}_2) \quad (32)$$

derived directly from Eq. 30.

In Figure 2 we plot the radial part of the wave functions $u_l(r)$ used to build the projector for $SrVO_3$, $LaVO_3$ and Cerium. In transition metal oxides we project to the $3d$ orbitals of Vanadium, and in Cerium metal we projected to Ce-$4f$ orbitals.

The projector, when written in Kohn-Sham basis, is orthonormalized locally, so that the resulting local Green's function has correct normalization, i.e., $\lim_{i\omega \to \infty} G_{local}(i\omega) = \frac{1}{i\omega} + \cdots$.

Notice that we do not remove the rest of the states from consideration, as is customary done when low energy Hubbard models are build. We just treat the above defined "correlated" states dynamically, and the rest of the states statically within LDA, hence we allow strong hybridization between "correlated" states and the itinerant states.

SCREENED COULOMB REPULSION OF YUKAWA FORM

It is noted in the manuscript that there is a unique relationship between the inverse screening length λ and the Hubbard interaction U. Moreover, for constant screening length λ, Hund's coupling as well as higher order Slater integrals, are uniquely determined either from $U \equiv F^0$ or from λ. Here we derive the precise relationship between Slater integrals and screening λ.

The matrix elements of the screened Coulomb repulsion (of Yukawa form) in the orbital basis defined above are

$$U_{m_1 m_2 m_3 m_4} = \int d^3 r \int d^3 r' \left(\frac{u_l(r)}{r}\right)^2 \left(\frac{u_l(r')}{r'}\right)^2 Y^*_{lm_1}(\hat{\mathbf{r}}) Y_{lm_4}(\hat{\mathbf{r}}) Y^*_{lm_2}(\hat{\mathbf{r}}') Y_{lm_3}(\hat{\mathbf{r}}') \frac{e^{-\lambda|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \tag{33}$$

There exist a well known expansion of Yukawa interaction in terms of spheric harmonics Y_{km}, which reads

$$\frac{e^{-\lambda|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = 4\pi \sum_k \frac{I_{k+1/2}(r_<) K_{k+1/2}(r_>)}{\sqrt{r_< r_>}} \sum_m Y^*_{km}(\hat{\mathbf{r}}) Y_{km}(\hat{\mathbf{r}}') \tag{34}$$

Here $r_< = min(r, r')$, $r_> = max(r, r')$, I and K are modified Bessel function of the first and second kind. Inserting this expression into Eq. 33, we get

$$U_{m_1 m_2 m_3 m_4} = \sum_k \frac{4\pi}{2k+1} \langle Y_{lm_1} | Y_{km_1-m_4} | Y_{lm_4} \rangle \langle Y_{lm_2} | Y^*_{km_3-m_2} | Y_{lm_3} \rangle$$
$$\times (2k+1) \int_0^\infty dr \int_0^\infty dr' u_l^2(r) u_l^2(r') \frac{I_{k+1/2}(\lambda r_<) K_{k+1/2}(\lambda r_>)}{\sqrt{r_< r_>}}. \tag{35}$$

Hence, the screened Coulomb interaction has the Slater form with the Slater integrals being

$$F^k = (2k+1) \int_0^\infty dr \int_0^\infty dr' u_l^2(r) u_l^2(r') \frac{I_{k+1/2}(\lambda r_<) K_{k+1/2}(\lambda r_>)}{\sqrt{r_< r_>}}. \tag{36}$$

This is a product of two one-dimensional integrals and is very easy to efficiently implement.

It is clear from Eq. 36 that λ uniquely determines all F^k's, and furthermore, even one Slater integral (F^0) uniquely determines λ. This is because F^k are monotonic functions of λ and take the value of bare F^k at $\lambda = 0$ and vanish at large λ. Hence given F^0, the screening length λ is uniquely determined, and hence other higher order F^k are uniquely determined as well.

Unfortunately, the screening in solids can not be predicted to very high accuracy yet, hence, instead of computing U we rather fixed it to $U = 10\,\text{eV}$ (a good approximation for most of transition metal oxides - see Ref.[2]). In this case, we can calculate parameter λ, and Hund's interaction J. For the two materials studied here, we got

SrVO$_3$:

$$\begin{aligned} U(\lambda = 0) &= 21.5\,\text{eV}, & J(\lambda = 0) &= 1.23\,\text{eV} \\ U(\lambda = 0.676/r_B) &= 10\,\text{eV}, & J(\lambda = 0.676/r_B) &= 1.13\,\text{eV} \end{aligned} \tag{37}$$

LaVO3:

$$\begin{aligned} U(\lambda = 0) &= 22.3\,\text{eV} & J(\lambda = 0) &= 1.27\,\text{eV} \\ U(\lambda = 0.734/r_B) &= 10\,\text{eV} & J(\lambda = 0.734/r_B) &= 1.16\,\text{eV} \end{aligned} \tag{38}$$

Ce:

$$\begin{aligned} U(\lambda = 0) &= 23.6\,\text{eV} & J(\lambda = 0) &= 0.923\,\text{eV} \\ U(\lambda = 1.512/r_B) &= 6\,\text{eV} & J(\lambda = 1.512/r_B) &= 0.719\,\text{eV} \end{aligned} \tag{39}$$

As is clear from these results, the Hubbard interaction in transition metal oxides is reduced from unscreened value for roughly factor of two, while the Hund's term is reduced for approximately 10%. In Cerium, U is screened twice as much, while J is screened for roughly 20%. This small screening of Hund's term, as compared to Hubbard term, is well known from studies of multiplets in lanthanides and actinides.

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[1] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. of Mod. Phys. **68**, 13 (1996).
[2] K. Haule, T. Birol, and G. Kotliar, Phys. Rev. B **90**, 075136 (2014).
[3] K. Haule, C.-H. Yee, and K. Kim, *Phys. Rev. B* **81**, 195107 (2010).