Title of the project

Outline: The coming green energy transition underscores the need for the discovery of materials with sustainability applications. Density functional theory (DFT) has long served as a computational workhorse for materials science feeding the electron density as the fundamental quantity. Ad for pads resole versus AA cheap transpiration al scaling of $O(N^3)$, where N is the number of electrons in the system, DFT treats the repulsive interactions between elections with an exchange corporation functional which is often approximated; this functional may work for certain classes of systems, but not others. A potential solution is the application of green's functions in many body perturbation gave. Central to this is the Dyson equation

$$G = G_0 + G_0 \Sigma G \tag{1}$$

an which the queen's function for the fully interacting system G is related to the noninteracting queen's function G_0 through the self-energy Σ. In the comment GW pronation, it is assumed that the self energy Σ takes the form iGW, where W is the screened Coulomb interaction. Therefore, the self energy is a functional of the interacting greens function (i.e. $\Sigma = \Sigma[G]$.) and the dasen equation must be solved self consistently. An exact closed set of equations known as the Hedin equations, which are represented schematically in figure 1, is used to solve equation **??** in practice, with the gut of proximate ignoring the vertex corrections Γ, which described the interaction between elections and halls.

The most basic approximation is $G_0 W_0$, which makes the assumption that $\Sigma \approx iG_0 W_0$, resulting in a computational scaling of $O(N^4)$. However, $G_0 W_0$ exhibits an undesirable strong starting point dependence on the noninteracting queens function meaning the accuracy of your GW catenation is at the mercy of the quality of G_0, which is usually taken as a trigger DFT calculation. On the other hand, the fully self-consistent GW (scGW) approach aluminate the dependence on the starting point. However, this comes with a higher $O(N^6)$ cost and often does not offer much improvement over $G_0 W_0$ for systems with strongly copulated electrons.

It is thought that the reason for this inaccuracy is the neglect of vortex corrections in the GW approximation, but by inclusion of these computations can become prohibitively expensive. The inadequacy of the GW approximation can be attributed to the fact that it relies expansion of the Dyson equation in terms of the strength of the perturbation:

$$G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \dots. \tag{2}$$

Each additional term carves with it an additional power of the interaction strength, as described by W. This means that the GW approximation is accurate for systems with weekly calculated elections, were it is reasonable to expand the Dyson equation in the colum interaction, since this is small. However, for strongly correlated systems this is not a reasonable thing to do.

Mori-Zwanzig Equation as an Alternative Despite the deficiencies noted above, there is interest in exploring alternative formulations of many-body perturbation theory using Green's functions. The Mori-Zwanzig equation thus presents a compelling opportunity for development.

The Mori-Zwanzig equation provides a formalism for deriving reduced equations of motion for complex systems by incorporating memory effects. It is expressed as:

$$\frac{d}{dt}e^{tL}u(0) = e^{tL}PLu(0) + \int_0^t e^{sL}PLe^{(t-s)QL}QLu(0)\,ds + e^{tQL}QLu(0) \tag{3}$$

where L is the Liouville operator, and $u(t)$ is the observable function.

Comparison with GW Approximation While the Mori-Zwanzig equation is traditionally less popular in quantum many-body theory compared to approaches like GW, its unique treatment of memory effects provides a potential pathway for handling strongly correlated systems without relying on Wick's theorem. This

approach can be advantageous in capturing non-Markovian dynamics inherent in many-body systems.

The Mori-Zwanzig framework, through its incorporation of projection operators and memory functions, could offer a systematic way to incorporate higher-order correlations and interactions, potentially leading to new insights into the electronic properties of materials. Despite its computational complexity and challenges in systematic renormalization, recent advancements in combinatorial Mori-Zwanzig theory have introduced novel non-perturbative expansions that are promising for capturing complex many-body interactions.

Both G_0W_0 and scGW have their unique advantages and challenges. G_0W_0 is computationally accessible and effective for a broad range of systems, particularly when an accurate starting point is available. In contrast, scGW is more robust in challenging systems but at a significant computational expense. Understanding the balance between computational feasibility and accuracy is crucial as we advance toward predictive materials design.

In summary, the GW approximation, with its variants and enhancements through vertex corrections, plays a pivotal role in advancing theoretical spectroscopy and electronic structure calculations, providing critical insights into the properties of materials and guiding the development of novel applications. The Mori-Zwanzig equation, with its potential to address non-Markovian effects, presents an exciting avenue for future exploration as an alternative or complementary approach to the GW method.

Motivation and Intellectual Merit: Describe the research background and intellectual merit of the project.

Research Plan The proposed plan for the research project you are describing. Here is some math:

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi G T_{\mu\nu}.$$

This is a note to myself about something to do later. And here is an example citation [**?**]. Let's cite another paper because we're good scientists [**?**].

Broader Impacts This is the section where you describe broader impacts.