

In electronic structure for realistic systems, the equations governing the observable properties of molecules, materials and their reactions are known. However, these equations are unfortunately insoluble in general, and their approximate, yet accurate and scalable numerical solution has long been sought after. Progress in this field holds the promise of widespread impact in the predictive computational determination of molecular properties, unique insight into reaction pathways and intermediates, the inverse design of materials, and much more. Innovative and emerging methods for the numerical solution to these equations have allowed theoreticians to model ever larger systems, with increasingly reliable accuracies.

However, in systems where the electronic correlation is strong and the standard approach of density functional theory is uncertain, the resolution necessary for predictive accuracy, key insights and the guiding of experimental design are missing. These arise in an increasingly documented set of cases, from bond-breaking, heterogeneous catalysis, to electronic excitations. Here we look towards the prospects and directions in post-mean-field electronic structure theory, discussing some of the main emerging paradigms for realistic electronic structure, in both molecular and materials settings, for these more demanding electronic structure cases. These directions will be set in the context of outstanding challenges, current limitations and experimental needs in the field, and will be focused into the following four research themes:

- Novel perturbative and variational methods for stronger correlations
- Stochastic and low-scaling techniques
- Extended systems
- Correlation in extended systems

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BCS correlation in real space
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