



## Sommerfeld Theory Colloquium

**Prof. Ali Alavi**

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### **Can we tame the electronic Schrödinger equation?**

One of the major problems of computational chemistry is the ab initio prediction of energies and properties of molecules. The electronic Schrödinger equation provides the in-principle solution, but because of intrinsic difficulties associated with the singular and long-ranged Coulomb interaction, this remains an extremely challenging task numerically. Here we outline a formalism called transcorrelation which provides a route out of the difficulties, whilst itself creating new problems (which have stumped the community for decades). We outline our work of the past few years in tackling these new problems, and show that the formalism has the potential to transform our ability to solve the Schrödinger problem in a general manner. In particular, by eliminating the Coulomb singularities, we show we can achieve both basis-set converged results, as well as thermodynamic limit results, with far fewer resources and less sophisticated many-body theories. Prospects to extend this methodology in the context of quantum computing will also be mentioned.

**Wednesday, 19 June 2024, 15:15h, Room A348, Theresienstr. 37/III**

Dr. Christian Schilling