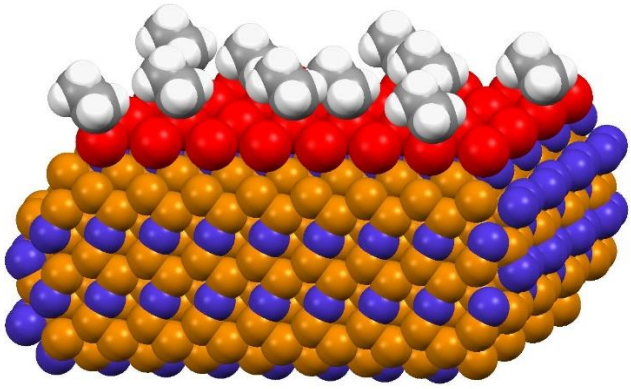
**Center for Complex Materials from First Principles (CCM)**
**EFRC Director: John P. Perdew**
**Lead Institution: Temple University**
**Class: 2014 – 2020**

***Mission Statement****: To develop, test, apply, and experimentally validate improved methods of electronic structure calculation for both simple and complex materials (including quantum materials).*

BACKGROUND: EFRC CCM is an extension of the 2014-2018 *Center for the Computational Design of Functional Layered Materials (CCDM)*, which demonstrated that computationally-efficient first-principles density functionals can work well not only for simple materials but even for many complex ones.

CCM brings together world-class scientists from different disciplines to tackle problems in the field of complex materials in new ways. To this end, CCM integrates state-of-the-art **Theory (Thrust 1)** with **Modeling and Computation (Thrust 2)** and **Experiment (Thrust 3)** to enable materials property predictions that are linked to **Experiment (Thrust 3)**, to accelerate the rate of progress on complex (including quantum) materials. Integration of the three thrusts is further enhanced by cross-cutting activities of **Forum A: Properties** and **Forum B: Applications.**

CCM will develop, test, apply, and experimentally validate improved methods of electronic structure calculation for both simple and complex materials. More accurate but still computationally efficient methods will be useful to many scientists. In particular, these methods will increase the reliability and expand the range of high-throughput computational searches for materials with desired properties. Because they will be developed from first principles, the new methods will be reliable and widely predictive. Planned tests and applications include the layered and two-dimensional materials, the cuprate high-temperature superconducting materials, water at interfaces, catalysis, and materials synthesis.



A material is defined by its chemical composition and structure. Complex materials are those in which small and difficult-to-predict energy differences per atom can imply large qualitative changes in other properties, leading in many cases to rich phase diagrams (and often to enlarged unit cells). Easy switching between phases can be exploited for some practical applications. For other applications, the relative stability of simple materials is advantageous. There is of course a continuum from simple to complex materials. Predictive theoretical methods should apply to both kinds of materials (and to surfaces, clusters, and molecules), and thus must be based upon the first principles of quantum mechanics. These

methods should range from the more highly-accurate ones that can provide benchmarks to the more computationally-efficient ones that permit wider searches over the enormous space of possible materials. Complex materials include the quantum (e.g., low-dimensional and cuprate) materials, but also more familiar ones like ice (or other molecular crystals) and liquid water at interfaces. CCM will develop some benchmark methods, such as a coupled cluster or random phase approximation, but will mainly focus on the more computationally-efficient density functional methods. Better density functionals for complex materials will imply better theoretical descriptions of interfaces and catalysis, and new targets for materials synthesis.

Density functional theory can in principle determine the exact ground-state properties for interacting electrons subject to static scalar external (possibly spin-dependent) potentials, via solution of self-consistent one-electron equations. Accessible properties include electron spin densities, total energy, fundamental energy gap in a generalized Kohn-Sham implementation, and forces on nuclei. Within the adiabatic and classical-nuclei approximations, this theory also determines vibrational properties of nuclei, and serves as a foundation for *ab initio* molecular dynamics. Many-body effects are taken into account, not through a computationally-expensive correlated wavefunction, but through a density functional for the exchange-correlation energy, whose functional derivative is an exchange-correlation potential. This functional is "Nature's Glue", providing most of the binding between atoms in a material or molecule. The exact functional is well-defined but un-computable in practice. Simple approximations to it however provide a practical and often usefully accurate way to predict binding energies, equilibrium geometries, equations of state, phase transitions, vibrational frequencies, etc., for many materials or molecules.

Until recently, accurate non-empirical density functional calculations were only possible for simple materials. Work done in CCDM showed that density functional approximations constructed to share many properties of the exact functional (exact constraints) can be accurate even for some complex materials. CCM will extend this work by making better functionals, then validating and applying them more widely.

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