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

RESEARCH PLAN

CCM will develop more accurate but still computationally-efficient density functionals from first principles, testing and applying them to layered and two-dimensional materials, water at interfaces, catalysis, and cuprate high-temperature superconducting materials.

http://efrc.cst.temple.edu/