Ab initio periodic quantum chemistry

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Ab initio wavefunction-based quantum chemistry represents a tantalizing alternative to density functional theory for problems in materials science, due to the former's ability to achieve high accuracy with systematic improvability. I will give an overview of our group's research efforts in this direction, describing theoretical and methodological developments at the periodic Hartree-Fock level (especially concerning atom-center basis functions) and post-Hartree-Fock level (especially perturbation theory and coupled-cluster theory), as well as connections to popular Green's function-based techniques. I will present applications to periodic crystals—including insulators, semiconductors, and metals—as well the use of quantum embedding techniques for aperiodic problems, such as defects in crystals or molecules on surfaces.