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A New View of the Kondo Effect from an Ab Initio Embedded Configuration Interaction Theory

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Over the past decade, we have been developing an ab initio theory to describe localized correlated many-electron states in condensed matter. This theory embeds a correlated quantum chemistry description into surroundings described by periodic density functional theory (DFT). Recent technical advances in the theory include: (i) implementation of ultrasoft pseudopotentials (USPPs) in a consistent manner across all levels of theory (periodic DFT, CASSCF, and CI), (ii) self-consistent updates of the density of the total system, thereby allowing a fully-self-consistent embedding operator, and (iii) a multi-reference singles and double excitation CI (MRSDCI) treatment of electron correlation in the embedded region. Our current embedded configuration interaction (ECI) theory is now more efficient (via USPPs), less approximate (by use of self-consistent embedding potentials), as well as more accurate (via MRSDCI) than earlier versions that were based either on many-body perturbation theory or valence CI/CASSCF wavefunctions. The current version is now being used to study a variety of systems/phenomena where DFT is known to fail, due to either neglect of many-body effects or self-interaction artifacts. Time permitting, more than one example will be given of how the embedding theory is able to give a *qualitatively (as well as quantitatively)* different view of these systems/phenomena. We will focus on the Kondo effect, a long standing problem in condensed matter physics, which has not had a first principles solution until now. The Kondo effect refers to the observation of an anomalous resistivity minimum at low temperatures for materials containing magnetic transition metal impurities in nonmagnetic host metals. We will show that the ECI theory is able to capture the physics and offer a new view of this phenomenon, while periodic DFT and finite cluster quantum chemistry calculations do not.