MAR12-2011-003876

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Validation of Atomic, Molecular and Condensed Matter Calculations

ERIC SHIRLEY, NIST

The advances in calculational techniques have brought first-principles calculations to a state of frequently having their results for various physical properties agreeing will with measured results for the same properties. Validation of computational results can therefore be an important undertaking in the overall scheme of first-principles work. Along these lines, such validation does not refer to the appropriateness of approximations made in calculations which are necessary to have a practicable methodology. Rather, such validation refers to whether calculations are implemented correctly given whatever approximations one assumes. Three areas are to be discussed in turn to illustrate issues that may arise. These include density-functional total-energy calculations in atoms and ions, in which as many as four atomic-structure programs were tested (and corrected) to permit reasonably high-precision comparisons of results. Second, calculations of dielectric properties and excitation spectra of solids shall be discussed, to illustrate the myriad of choices one might be required to make in terms of approximations, and how various approximations' results can only be compared if numerical methodologies used in conjunction with the respective approximations are sufficiently similar. Third, as a point of reference, brief consideration shall be given to the progress in the calculational validation area made within the quantum chemistry community.