Department of Physics and Materials Science

SEMINAR

Like Vibrational Zero-Point Energy for Atoms

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Abstract: Most computations in quantum chemistry are done using the Born-Oppenheimer approximation and non-relativistic quantum mechanics. To obtain accurate energetics, both approximations require corrections. The simplest correction for the B-O approximation is vibrational zero-point energy and is made routinely. Two relativistic corrections are sometimes applied, for orbital contraction and for spin-orbit coupling (SOC). Both corrections are routine in careful work. However, the correction for SOC is based upon a simple model that breaks down for many atoms and molecules. This problem is not widely recognized, and improved corrections are not yet available.

Bio: My thesis work at Caltech dealt with the gas-phase chemistry of transition-metal ions, primarily using ion-cyclotron resonance mass spectrometry (under J. L. Beauchamp), but also ab initio theoretical methods (under W. A. Goddard III). I moved to Maryland in 1991 for a postdoc at NIST, measuring the spectra of free radicals using resonance-enhanced multiphoton spectroscopy (under J. W. Hudgens). When the postdoc ended, I was hired into a permanent position as a theoretician in the Chemical Kinetics and Thermodynamics Division at NIST. I am currently in the Chemical Sciences Division.

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