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Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy

By Langhoff, S.

Book Condition: New. Publisher/Verlag: Springer Netherlands | The theoretical chemist is accustomed to judging the success of a theoretical prediction according to how well it agrees with an experimental measurement. Since the object of theory is the prediction of the results of experiment, that would appear to be an entirely satisfactory state of affairs. However, if it is true that "the underlying physical laws . for the whole of chemistry are . completely known" (1), then it should be possible, at least in principle, to predict the results of experiment more accurately than they can be measured. If the theoretical chemist could obtain exact solutions of the Schrodinger equation for many-body systems, then the experimental chemist would soon become accustomed to judging the success of an experimental measurement by how well it agrees with a theoretical prediction. In fact, it is now possible to obtain exact solutions of the Schrodinger equation for systems of a few electrons (2-8). These systems include the molecular ion H_2^+ , the molecule H_2 , the reaction intermediate $H-H-H$, the unstable pair $H-He$, the 2 stable dimer He_2 and the trimer He_3 . The quantum Monte Carlo method used in solving the time-independent Schrodinger equation for these systems is exact in that it requires no physical or mathematical assumptions beyond those of the Schrodinger equation. As in most Monte Carlo methods...



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