Modeling energy states of lithium dimers with the Born-Oppenheimer approximation COLLIN LUECK, University of Dallas — To obtain energy eigenstates of a two-atom system, it is necessary to separate the wavefunction of the system into nuclear and electronic components. In an adiabatic approximation, the nuclear component is a function of internuclear distance, and the electronic component is a function of electron-nuclear distance. When this approximation is used with the Numerov numerical method for plotting wavefunctions and a Distributed Approximating Function for finding energy eigenstates, it allows for plotting the energies of uncoupled states. However, more elegant and accurate solutions exist. Using a diabatic approximation, in which the wavefunctions of the nuclei are functions of the nuclear separation as well as parametric functions of the electronic motion, much more accurate energy eigenvalues are obtained. This method, when combined with a function to prevent crossings of the energy eigenstates using Clebsch-Gorden coefficients, yields a much more realistic energy plot and a deeper understanding of the two-atom system.

Collin Lueck
University of Dallas

Date submitted: 06 Feb 2010   Electronic form version 1.4