

PHYSICS-GUIDED CURVE FITTING FOR POTENTIAL-ENERGY FUNCTIONS OF DIATOMIC MOLECULES

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In ab initio calculations of diatomic spectroscopy, discrete points are typically computed along the potential energy curve. The points are fitted to a continuous function, such as a polynomial, a Morse function, or a spline, so that ro-vibrational energy levels can be computed and conventional constants extracted. The choice of fitting function is arbitrary and affects the results, which is undesirable in predictive work. Here we suggest using lower-level theory to create a dense, high-resolution grid, to be used as a guide. Instead of fitting the sparse, high-level data directly, the energy differences between the high-level points and the guiding potential are fitted. This simple strategy reduces the uncertainty from the choice of fitting function, yielding more precise predictions.