AUTOSURF: A CODE FOR AUTOMATED CONSTRUCTION OF POTENTIAL ENERGY SURFACES

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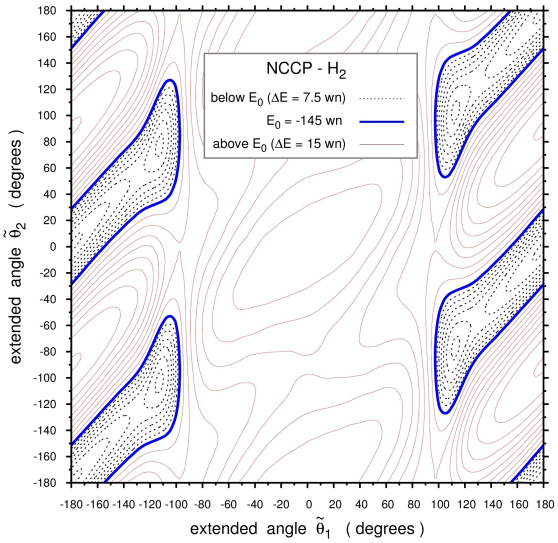
The potential energy surface (PES) of a molecular system constitutes a cornerstone for every theoretical study of spectroscopy and dynamics. We describe here our general code for the automated construction of PESs for van der Waals (vdW) systems composed of two (rigid) fragments. The AUTOSURF suite is designed to completely automate all of the steps and procedures that go into fitting various classes of PESs. The algorithms are based on the local interpolating moving least squares (L-IMLS) methodology, and have many advanced features such as options for data-point placement, and iterative refinement. We have interfaced this fitting approach to popular electronic structure codes such as Molpro and CFOUR to automatically generate ab initio PESs for 3D (atom - general molecule) and 4D (linear molecule - linear molecule) vdWs systems. The niche of these algorithms is to obtain an interpolative representation of high-level ab initio energies with negligible (arbitrarily small) fitting error, enabling a broad community of non-experts in PES fitting methods to bridge electronic structure calculations and spectroscopic and dynamics research.



The code is demonstrated here by presenting PESs and analysis of the corresponding rovibrational bound states for 7 highly anisotropic "heavy-light" systems: C_6H^--H_2, HC_2NC-H_2, HNC_3-H_2, HC_5N-H_2, C_4H^--H_2, MgCCH-H_2, NCCP-H_2.