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Abstract: In this talk, the use of the neural network (NN) method with exponential neurons for directly fitting ab initio data to generate potential energy surfaces (PESs) in sum-of-product form will be discussed. The utility of the approach will be highlighted using fits of CS₂, HFCO, and HONO ground state PESs based upon high-level ab initio data. Using a generic interface between the neural network PES fitting, which is performed in MATLAB, and the Heidelberg multi-configuration time-dependent Hartree (MCTDH) software package, the PESs have been tested via comparison of vibrational energies to experimental measurements. Future directions will be highlighted.