AB INITIO CALCULATIONS OF THE LOW LYING $^2\Pi$ STATES OF NO

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The NO molecule has too many electrons. The ground electronic state is of $^2\Pi$ symmetry, and can only form a double bond. The valence electronically excited $^2\Pi$ states are many, and can only form single bonds or are repulsive. In contrast, the NO^+ molecule can form a triple bond. Thus there are strongly bound Rydberg states in NO, and these give rise to a myriad of avoided crossings in the Born-Oppenheimer (BO) picture. These crossings are very troublesome, for example the B,C avoided crossing occurs at $v = 3$ for the C state, and this causes vibrational calculations using the BO picture to be impossible. In this work we show how the BO picture can be de-perturbed in *ab initio* calculations without resorting to a diabatic transformation starting from the asymptotic region.