Application of the stabilization method to the CO2 anion potential surface

Dr Rodney J. Bartlett

Alexandre P. Bazanté

We have used the stabilization method to calculate the resonance parameters of the CO2 anion shape resonance along the symmetric stretching and bending modes. The resonant character of the CO2 temporary anion makes its study difficult for it requires an appropriate description of its continuum component. Ab initio Coupled Cluster theory and its equation of motion family of methods offers an accurate description of anions, even near the ionization threshold. The stabilization method used in conjunction with an analytic continuation in a diffuse basis set with even-tempered functions has been very effective describing resonance parameters of isolated shape resonances in diatomic molecular anions and offer an alternative to approaches such as complex absorbing potential equation of motion coupled cluster. In this paper, we show that the stabilization method performs as well on a more complex shape resonance such as the CO2 anion, which includes vibronic coupling of at least three anion states.