

ACCURATE AB INITIO SPECTROSCOPY

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The future of ab initio spectroscopy is very bright. By including extrapolations to the basis set limit, an accurate electron correlation treatment, accurate core-valence interaction, relativity and Born-Oppenheimer breakdown, and accurate nuclear dynamics, it is possible to obtain results of sub wavenumber accuracy for small molecules. In the present talk we will discuss applications of these techniques to CO, H₂O, and CH₄.