Exploring the Limits of Ab Initio Electronic Structure Methods: AlF Case Study

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The AlF molecule is a good candidate for laser cooling experiments and subsequent precision measurements to test fundamental laws of physics. We analyzed the limits of current state-of-the-art electronic structure methods in reproducing the spectroscopic properties of AlF. In order to do this, we developed a scheme for systematically estimating the uncertainty of theoretical computations and found that quantum electrodynamic and non-adiabatic effects are much larger than the resolution of a typical spectroscopic experiment.