ATOMIC PROPERTIES FROM ELECTRONIC STRUCTURE: $X^1\Sigma^+ CaF^+$

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- Purpose: Compare methods of obtaining atoms-in-molecules properties from electronic structure calculations and spectroscopy.
- Spectroscopic connection: Rydberg penetrating states and shape resonances see the atoms, non-penetrating states see molecules. Clusters see both.
- Scope: Ca and F in CaF+, and by extension, Ca and F in other bonded and non-bonded environments.
- Converting molecular properties to atomic models:
  1. Two point-localized models
     - dipole induction model with integer ionic charges
     - Hirshfeld local multipole model
- Data used:
  1. CCSD and CCSD(T) ab-initio calculations.
  2. Experimental values of $Q_1^2 - eQ_2$, and of dipole polarizability
- Result:
  1. Hirshfeld model connects long range multipole potential to atomic properties, and matches multipoles.
  2. Traditional dipole induction matches calc'd Q_1, Q_2, expt'l $Q_1^2 - eQ_2$, sensible atomic polarizabilities.