

# Overview of the major Cave impact in molecular quantum chemistry and beyond

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A continuously expanding range of models and applications for a diverse set of molecular coupling coefficients:

- electron transfer (**ET**) in diatomics (with Goddard et al)
- *1-dimensional* electron transfer (**ET**) in molecular systems: variational **maximization of dipole shift** (Generalized Mulliken Hush (**GMH**) with Newton et al)
- extension to general *3-dimensional* **ET** (with Subotnik et al, following Boys, Ruedenberg, et al)
- application to coupling governing spectral transitions: **maximization of transition moment** (with Stanton)