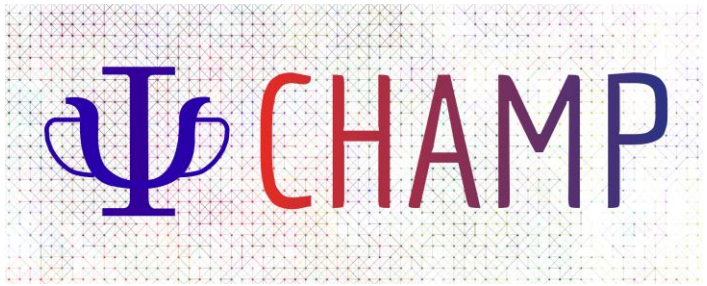


CHAMP : Cornell-Holland Ab-initio Materials Package

QMC suite of programs for accurate electronic structure calculations of molecular systems

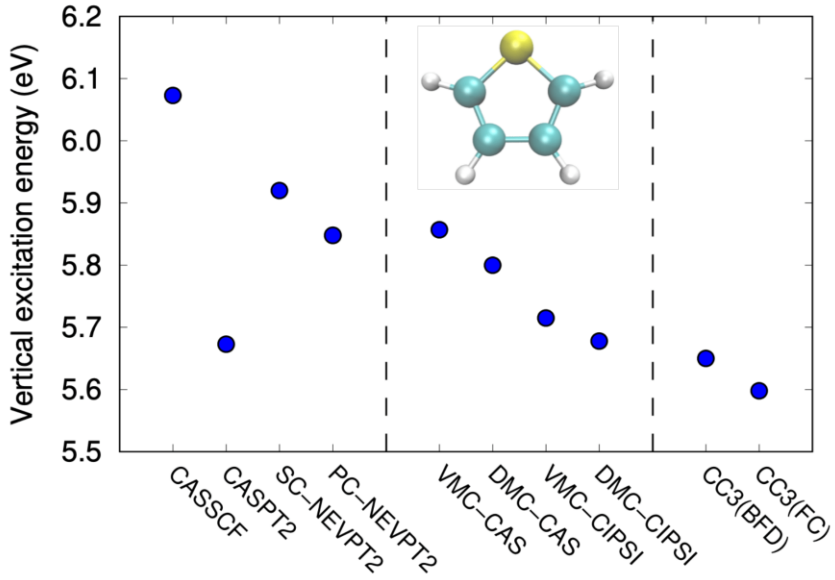
Stuart Shepard
University of Twente, The Netherlands

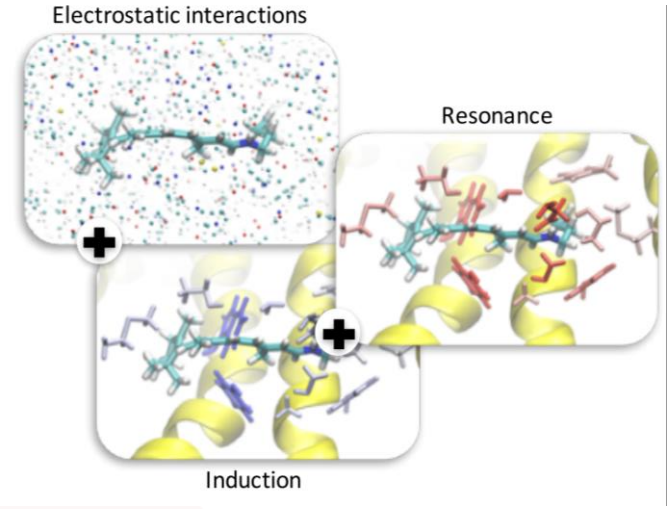
Excited States using CHAMP

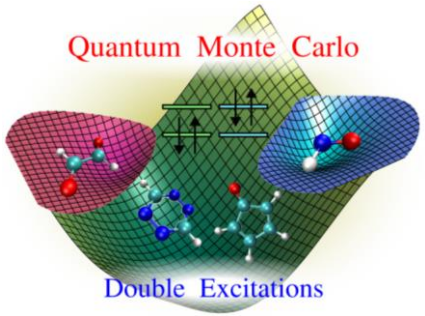
- VMC wave function optimization + DMC
  - Jastrow-Slater multi-determinant

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \mathcal{J}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \times \sum_i c_i \, D_i(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

  - Any symmetry
  - Embedding





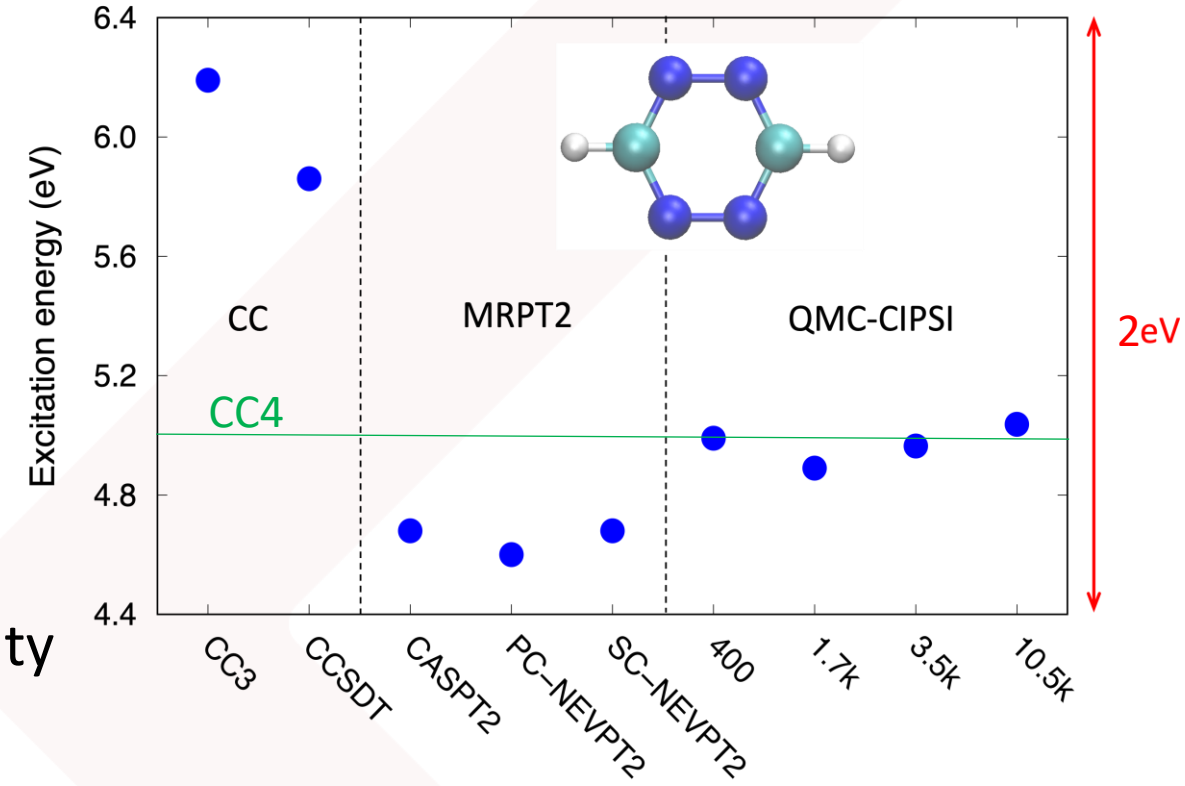


Accurate Double Excitations ➡ QP + CHAMP in action

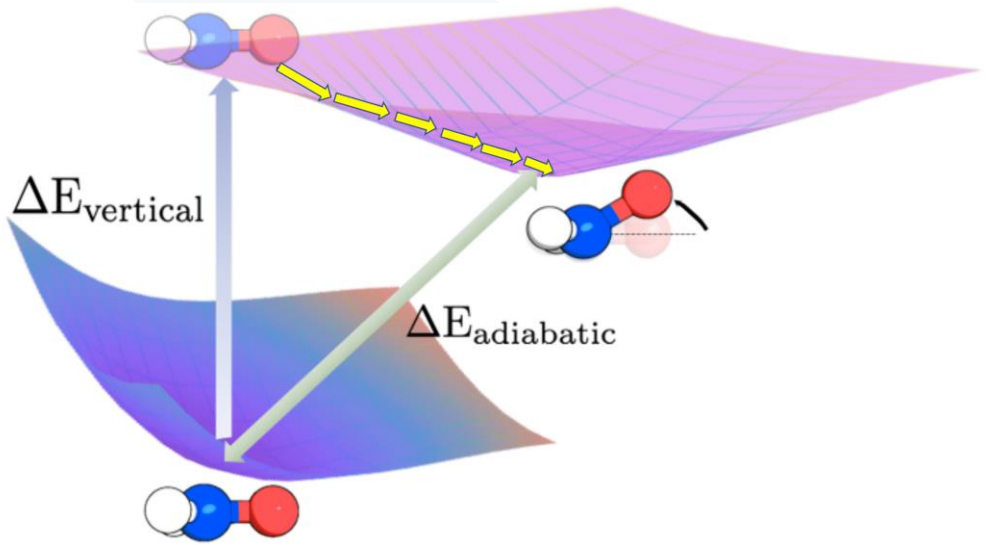
QP ➡ TREXIO ➡ CHAMP

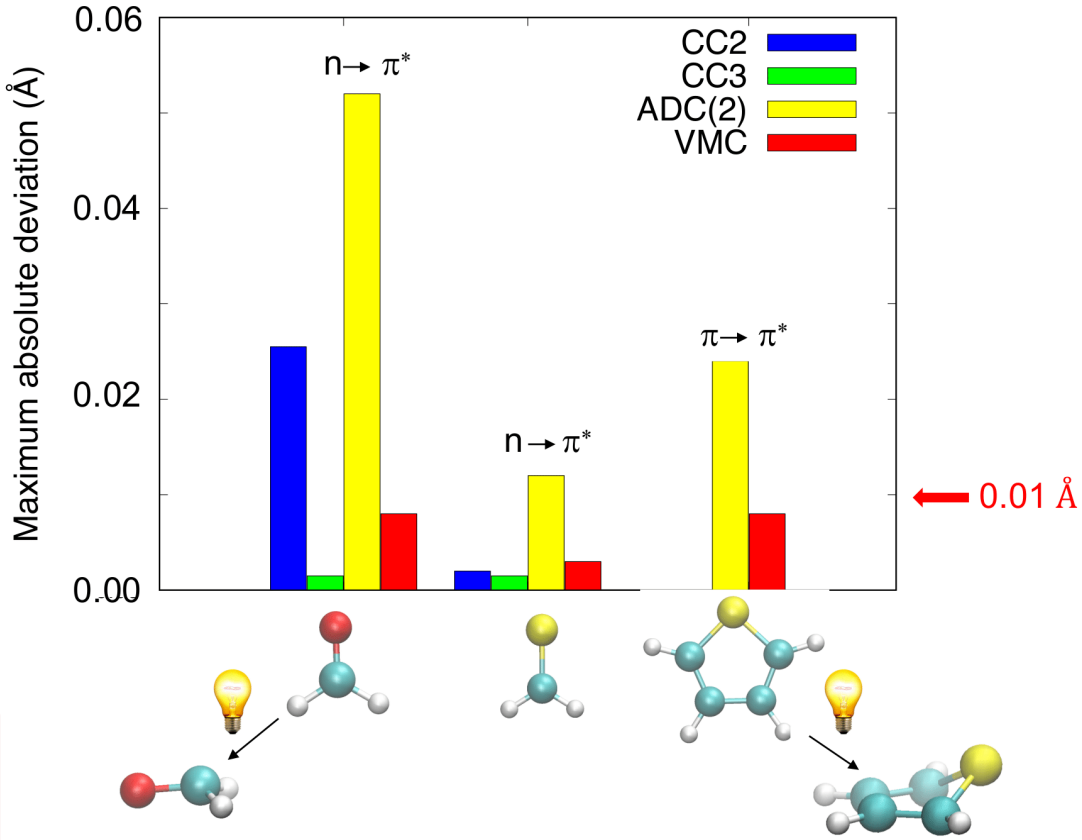
GAMESS ⬆ TREXIO

- States of same symmetry
- State-specific optimization with overlap penalty

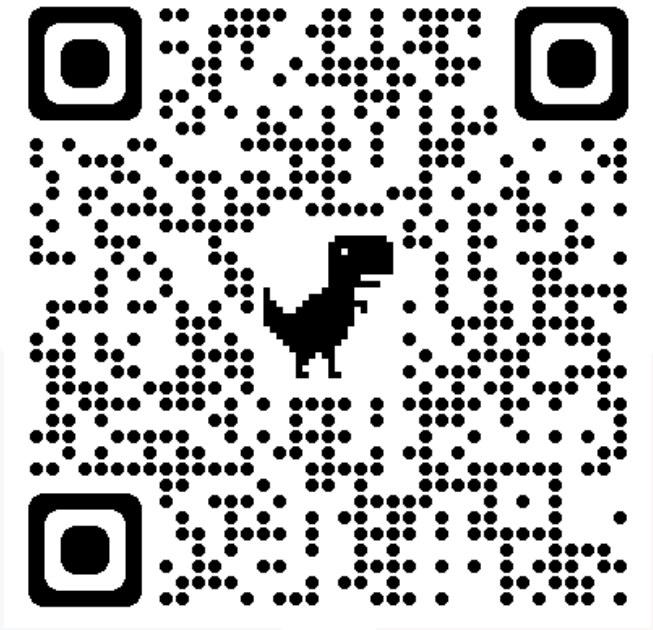


Example: Geometry Optimization in Excited State





Codes available on GitHub



Acknowledgements

Thank you!