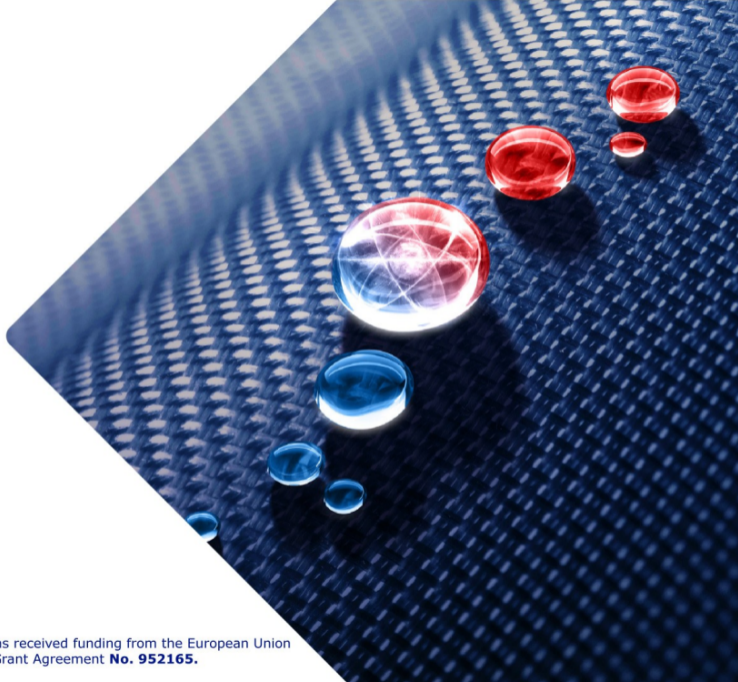


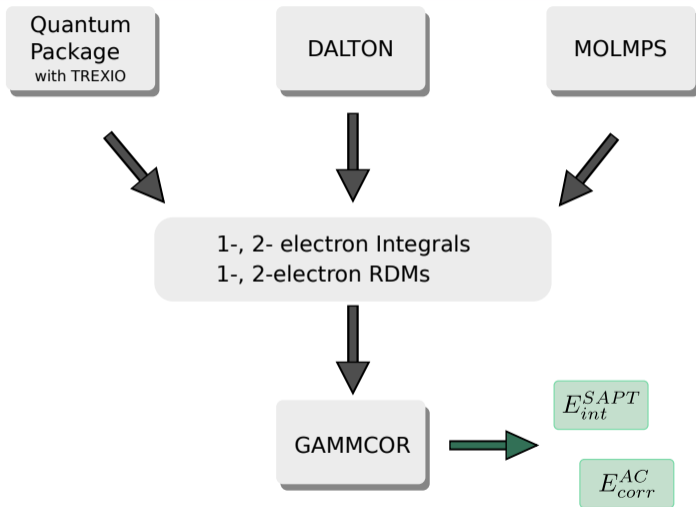
## GammCor Code Tutorial

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- 1 Install GammCor code
- 2 Run tests
- 3 Do exercises and discuss the results
  - SAPT (Quantum Package)
  - AC (MOLMPS)



EXERCISES



```
git clone https://github.com/michalhapka/trex_workshop2023.git  
or at Dragon  
cp /home/michalhapka/trex_workshop2023
```

GET THE CODE



```
git clone https://github.com/peralk/GAMMCOR.git  
cd GAMMCOR  
git checkout workshop2023
```

INSTALLATION  
GUIDE



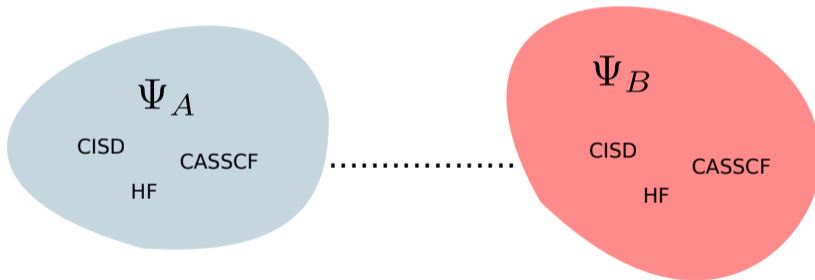
<https://qchem.gitlab.io/gammcor-manual/>

INSTALLATION  
AT DRAGON

```
module load intel/2021.1.1
git clone https://github.com/pernak/GAMMCOR.git
cd GAMMCOR
git checkout workshop2023
env FC=gfortran CXX=g++ CC=gcc cmake -S. -Bbuild -Cconfig_gnu
cd build
make -j 4
ctest -V
```

<https://qchem.gitlab.io/gammcor-manual>

$$E_{int}^{SAPT} = E_{elst}^{(1)} + E_{exch}^{(1)} + E_{ind}^{(2)} + E_{exch-ind}^{(2)} + E_{disp}^{(2)} + E_{exch-disp}^{(2)}$$



1 step

Quantum Package

 $\Psi_A \Psi_B$ 

two HDF5 files (one for each monomer)

2 step

 $\Psi_A \Psi_B$ 

GammCor

 $E_{int}^{SAPT}$



/trex\_workshop2023/SAPT

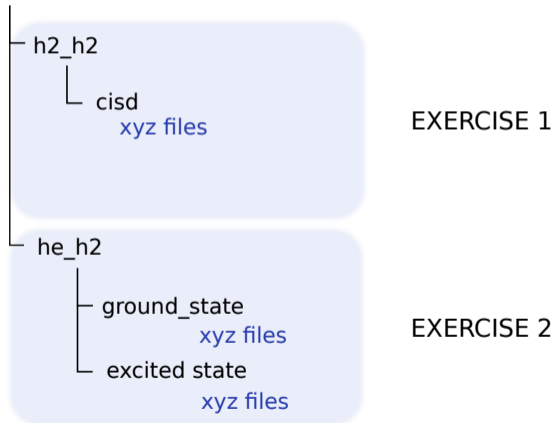


Table 1: Results of SAPT calculations for H<sub>2</sub>-H<sub>2</sub> dimer. Energy units are microhartree.

	$E_{\text{elst}}^{(1)}$	$E_{\text{exch}}^{(1)}$	$E_{\text{ind}}^{(2)}$	$E_{\text{exch-ind}}^{(2)}$	$E_{\text{disp}}^{(2)}$	$E_{\text{exch-disp}}^{(2)}$	$E_{\text{int}}^{\text{SAPT}}$
<i>R</i> = 1.44 a.u.							
HF	-62.29	89.96	-5.169	1.706	-154.2	6.911	-123.0
CISD	-52.70	88.98	-4.591	2.014	-151.5	6.111	-111.6
CAS(2,2)	-47.82	81.28	-4.030	1.637	-143.6	5.693	-106.8
CAS(2,8)	-52.61	88.43	-4.565	1.980	-151.7	6.094	-112.4
<i>R</i> = 7.20 a.u.							
HF	-185.4	445.0	-39.72	26.29	-320.6	33.55	-40.89
CISD	-47.28	210.0	-8.408	6.044	-165.6	10.45	5.193
CAS(2,2)	-44.87	201.1	-7.994	5.465	-161.1	10.15	2.748
CAS(2,8)	-47.17	209.4	-8.388	5.992	-165.9	10.43	4.335

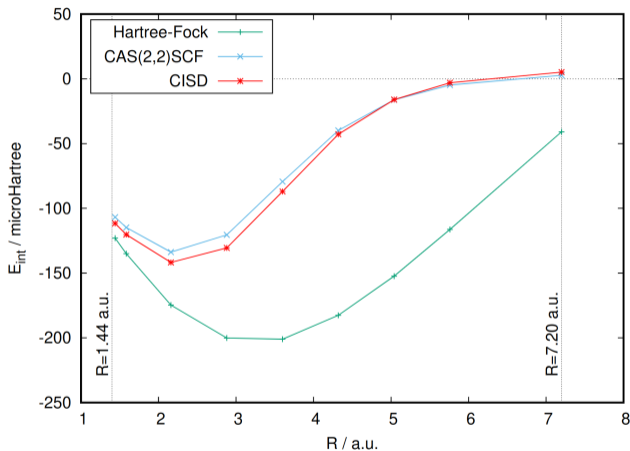


Figure 1: SAPT interaction energy curves for H<sub>2</sub>-H<sub>2</sub>.  $R$  denotes the covalent bond length in one the monomers.

Table 2: Results of SAPT(CISD)/aug-cc-pVDZ calculations for He-H<sub>2</sub> and He-H<sub>2</sub>\* dimers. Energy unit is millihartree.

	$E_{\text{elst}}^{(1)}$	$E_{\text{exch}}^{(1)}$	$E_{\text{ind}}^{(2)}$	$E_{\text{exch-ind}}^{(2)}$	$E_{\text{disp}}^{(2)}$	$E_{\text{exch-disp}}^{(2)}$	$E_{\text{int}}^{\text{SAPT}}$
ground state							
$R = 4.0$ a.u.	-1.103	5.740	-0.375	0.395	-0.956	0.114	3.816
$R = 6.6$ a.u.	-0.004	0.029	-0.001	0.001	-0.050	0.001	-0.024
excited state							
$R = 4.0$ a.u.	-0.558	0.776	-1.080	0.099	-1.076	-0.003	-1.843
$R = 6.6$ a.u.	-0.026	-0.060	-0.036	-0.003	-0.204	-0.005	-0.334

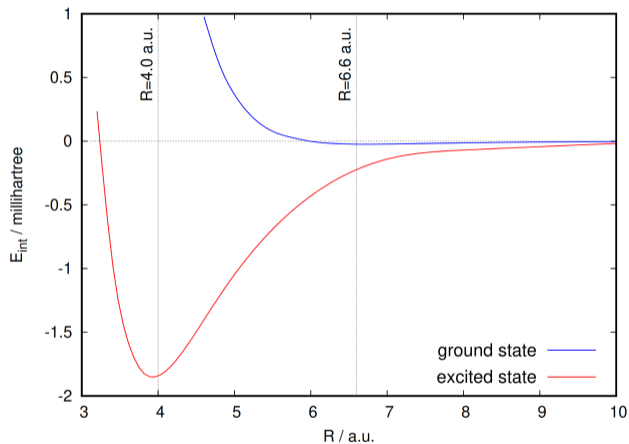


Figure 2: He-H<sub>2</sub> in T-shaped geometry.  $R$  denotes the distance between the He atom and COM of the H<sub>2</sub> molecule.

