Environment-controlled water adsorption at hydroxyapatite/collagen interfaces Supporting Information

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April 2021

1 CP2K input file

```
&FORCE_EVAL
  METHOD QS
  &DFT
  BASIS_SET_FILE_NAME BASIS_HYDRO
  POTENTIAL_FILE_NAME GTH_POTENTIALS
  &MGRID
  CUTOFF 400
  REL_CUTOFF 60
  &END MGRID
  &XC
  &XC_FUNCTIONAL
  &LIBXC
  FUNCTIONAL XC_MGGA_XC_B97M_V
  &END
  &END XC_FUNCTIONAL
  &vdW_POTENTIAL
  DISPERSION_FUNCTIONAL NON_LOCAL
  &NON_LOCAL
  TYPE RVV10
  PARAMETERS 6.0 0.01
  KERNEL_FILE_NAME rVV10_kernel_table.dat
  &END NON_LOCAL
  &END vdW_POTENTIAL
  &END XC
  &END DFT
```

where BASIS_HYDRO is
P TZVP-MOLOPT-GTH TZVP-MOLOPT-GTH-q5

O TZVP-MOLOPT-GTH TZVP-MOLOPT-GTH-q6
H TZVP-MOLOPT-GTH TZVP-MOLOPT-GTH-q1
Ca TZVP-MOLOPT-SR-GTH TZVP-MOLOPT-SR-GTH-q10
Ti TZVP-MOLOPT-SR-GTH TZVP-MOLOPT-SR-GTH-q12
S TZVP-MOLOPT-GTH TZVP-MOLOPT-GTH-q6
N TZVP-MOLOPT-GTH TZVP-MOLOPT-GTH-q5
C TZVP-MOLOPT-GTH TZVP-MOLOPT-GTH-q4

Table 1: Birch-Murnaghan fit results

Functional	E_0	B_0	B'	V_0
PBE	-6619.15786	0.028981	4.57	4503.30289
PBE-D3	-6620.72752	0.0294529	4.56	4470.08422
B97M_rV	-6615.70062	0.032584	4.70	4327.16438

2 Modeller input file adapted from online documentation

```
from modeller import *
from modeller.automodel import *    # Load the automodel class

log.verbose()

env = environ()
# directories for input atom files
#env.io.atom_files_directory = ['.', '../atom_files']

a = automodel(env,
        alnfile  = 'filename.ali' ,     # alignment filename
        knowns   = '3hr2',              # codes of the templates
        sequence = 'ColAlpha1I',
        assess_methods=(assess.DOPE,assess.GA341))           # code of the target


a.starting_model= 1
a.ending_model  = 10
 a.make()
```