

Supporting information for:

The Role of Polarons in Water Splitting: the Case of BiVO_4

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CP2K input file

Sample CP2K input file used to study the electron polaron in BiVO_4 at 0 K:

```
&FORCE_EVAL
  METHOD          Quickstep
  &DFT
    LSD
    CHARGE -1  ! for electron polaron
!   CHARGE  1  ! for hole polaron
    BASIS_SET_FILE_NAME  ~/cp2k/data/BASIS_MOLOPT
    POTENTIAL_FILE_NAME  ~/cp2k/data/GTH_POTENTIALS
    BASIS_SET_FILE_NAME  ~/cp2k/data/BASIS_ADMM
    BASIS_SET_FILE_NAME  ~/cp2k/data/BASIS_ADMM_MOLOPT
  &MGRID
    CUTOFF          600
    REL_CUTOFF       50
  &END MGRID
  &QS
    EPS_PGF_ORB      1.0E-32
    METHOD GPW
    EPS_DEFAULT       1.0E-10
    EXTRAPOLATION ASPC
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&END QS
&AUXILIARY_DENSITY_MATRIX_METHOD
  METHOD BASIS_PROJECTION
  ADMM_PURIFICATION_METHOD MO_DIAG
&END AUXILIARY_DENSITY_MATRIX_METHOD
&SCF
  SCF_GUESS RESTART
  EPS_SCF 1.0E-7
  MAX_SCF 50
&OT
  MINIMIZER DIIS
  PRECONDITIONER FULL_SINGLE_INVERSE
&END OT
&OUTER_SCF
  EPS_SCF 1.0E-7
  MAX_SCF 50
&END
&END SCF
&XC
  &XC_FUNCTIONAL
    &PBE
      SCALE_X 0.78
      SCALE_C 1.0
    &END PBE
    &PBE_HOLE_T_C_LR
      CUTOFF_RADIUS 5.0
      SCALE_X 0.22
    &END PBE_HOLE_T_C_LR
  &END XC_FUNCTIONAL
  &HF
    &SCREENING
      EPS_SCHWARZ 1.0E-6
      SCREEN_ON_INITIAL_P FALSE
    &END SCREENING
    &INTERACTION_POTENTIAL
      POTENTIAL_TYPE TRUNCATED
      CUTOFF_RADIUS 5.0
      T_C_G_DATA ~/cp2k/data/t_c_g.dat
    &END INTERACTION_POTENTIAL
    FRACTION 0.22
  &END HF
&END XC
&END DFT
&SUBSYS
  &CELL
    ABC [angstrom] 10.2985 10.2625 23.5003
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  &COORD
    Bi -0.0013370037 1.3453109792 7.3611915889
    Bi -0.0023121690 3.9112554287 4.3887239656
    Bi 2.5731527359 1.3452689432 10.2641209279
    Bi 2.5722827102 3.9112254670 1.4864109069
    Bi 5.1477445006 1.3453134928 7.3611740519
    Bi 5.1469674651 3.9113471498 4.3887584205

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Bi	2.5726788910	6.4761067201	10.2639870248
Bi	2.5721361450	9.0426833553	1.4862516598
Bi	5.1473210476	6.4761610623	7.3614553667
Bi	5.1467995558	9.0428136952	4.3887741291
Bi	7.7218600890	6.4761011048	10.2638821126
Bi	7.7214762410	9.0427665103	1.4861221065
Bi	-0.0013664172	1.3451579168	19.1113693352
Bi	-0.0023541609	3.9113541876	16.1388425962
Bi	2.5730808537	1.3451119405	22.0143037363
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Bi	5.1477952299	1.3451583054	19.1113102656
Bi	5.1470221167	3.9114310708	16.1388047417
Bi	7.7223390758	1.3450790876	22.0142183325
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Bi	-0.0024649814	9.0426191536	16.1390555923
Bi	2.5726182889	6.4762635370	22.0141162294
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V	-0.0022794994	9.0435601257	10.2570276102
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V	2.5724434894	9.0435923099	7.3681808193
V	5.1471863193	6.4785002055	1.4929162230
V	5.1469815265	9.0435870712	10.2570309208
V	7.7218441238	6.4784617325	4.3820821716
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V	-0.0019324731	3.9123209377	22.0072398270
V	2.5725710356	1.3471384003	16.1320795830
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V	-0.0022764101	9.0435796773	22.0071436372
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O	3.8762834840	2.0408512569	0.5775262127
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  AUX_FIT_BASIS_SET cFIT3
  POTENTIAL          GTH-PBE-q6
&END KIND
&KIND V
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  AUX_FIT_BASIS_SET cFIT10
  POTENTIAL          GTH-PBE-q13
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