Electronic Supplementary Material (ESI) for CrystEngComm.


# Supporting Information:

## Water coordination and dehydroxylation processes in defective UiO-66 type metal-organic frameworks

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## 1 Results of MD-simulations of three water coordinated to a Zr-O-Zr defect site

An NVT simulation starting from the G_3$H_2O$ state was first equilibrated during 5 ps (10000 steps), and from that point the Zr1-O1 and Zr2-O2 distances were monitored for more than 10 ps (see **Figure 3** for definitions of the distances). Fast oscilations between Zr-$OH_2$ and Zr-OH species were observed (**Figure S.1**) via a proton transfer reactions mediated by the oxygen atom O3. Furthermore, a histogram of the O3-O4 distances during this simulation is presented in **Figure S.2**.

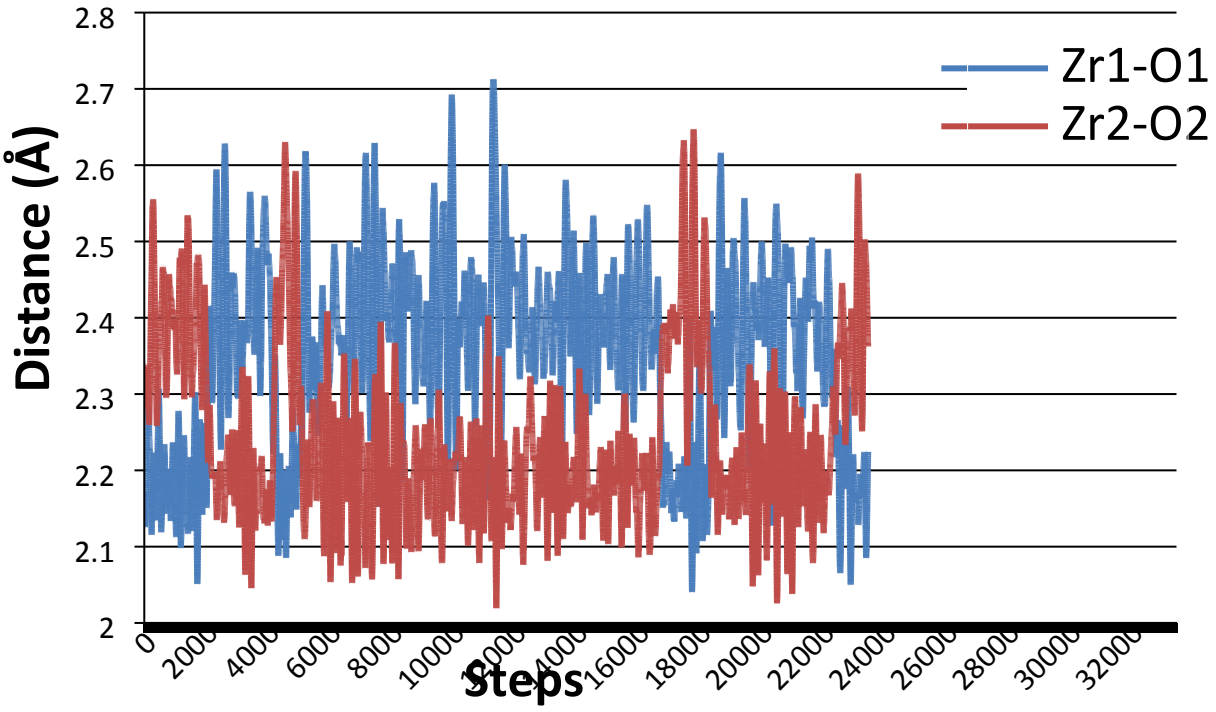



**Figure S.1**: Variation in Zr1-O1 and Zr2-O2 distances (in Å) originate from quick proton transfer reactions altering between different configurations of H-G_OH_2$H_2O$.

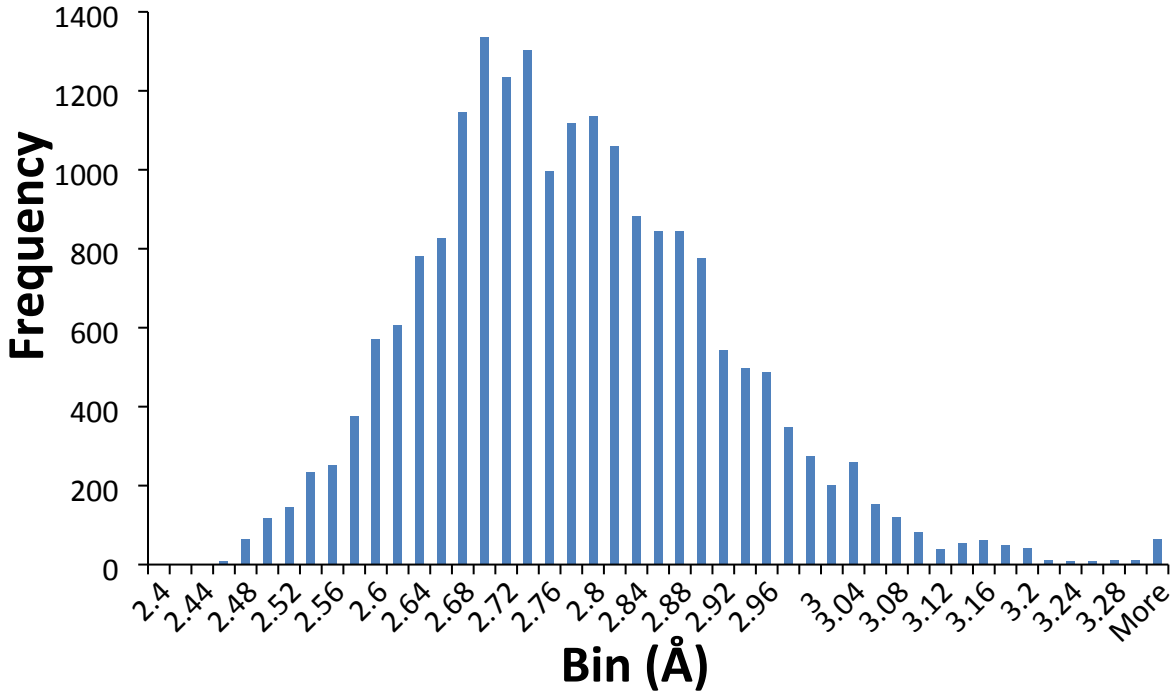



**Figure S.2**: Histogram of O3-O4 distances in Å has a maximum around 2.70-2.76 Å. The value corresponding with the left edge of the bin is given and the bin-size is 0.02Å.

# 2 Additional computational methodology

## 2.1 The bulk modulus

### Definition of bulk modulus

The energy E of a unit cell depends on the volume V of the unit cell, E(V). The bulk modulus B expresses the resistance to isotropic pressure, and relates to the second derivative of E(V) with respect to volume,

$$B = \left( V \frac{\partial^2 E}{\partial V^2} \right)_0$$

where the subscript 0 means that the expression is evaluated at the minimum energy point of the E(V) curve, corresponding to the volume $V_0$.

### Bulk modulus derived from calculations

**(1) From equation-of-state curve E(V):** The bulk modulus B may be derived from calculations by constructing the energy versus volume curve E(V), fitting a polynomial, and taking the second derivative in the minimum. This approach was successfully applied for the porous MIL-47(V) material, where, due to Pulay stress, the minimum needed to be located with the E(V) curve rather than with the standard conjugate gradient optimizer.[1]

**(2) From elastic tensor C:** Alternatively, the bulk modulus may be derived from the elastic tensor C, a symmetric 6x6 matrix in Voigt notation. When the harmonic approximation is assumed, the energy per unit cell may be expanded in terms of the strain tensor ε, which is a 6x1 vector in Voigt notation,

$$E = \frac{V_0}{2} \sum_{ij}^{6} C_{ij} \epsilon_i \epsilon_j$$

The elastic tensor C is constructed by first computing the clamped ion tensor C^clamped, where ion positions are scaled uniformly when the unit cell is strained without relaxing their position, and next correcting for the ion response. For this purpose, the extended Hessian is constructed, containing derivatives of the energy with respect to ion positions and strain.[1] The ion response is added by applying the Vibrational Subsystem Analysis (VSA)[2] with the strain coordinates as subsystem, and the 'responding' ion positions as environment coordinates, which results in the sought-for (relaxed ion) elasticity tensor C,

$$C = C^{\text{clamped}} - V_0 B^T H^- B$$

with $H^-$ the pseudo-inverse of the Hessian and B the off-diagonal block of the extended Hessian containing the mixed derivatives with respect to ion positions and strain.

The elastic tensor describes the strain response to a given stress. For an isotropic stress, the response is described by the Reuss bulk modulus $K_R$, which is computed by inverting C and then taking a weighted average of the upper left 3x3 subblock, so $K_R$ is the harmonic equivalent of B. The computation of $K_R$ is revised in detail in Ref. [1].

In addition, the Reuss shear modulus $G_R$ may be computed from the inverse of C as well.[1] This quantity describes the resistantance against unit cell deformation caused by shear stress.

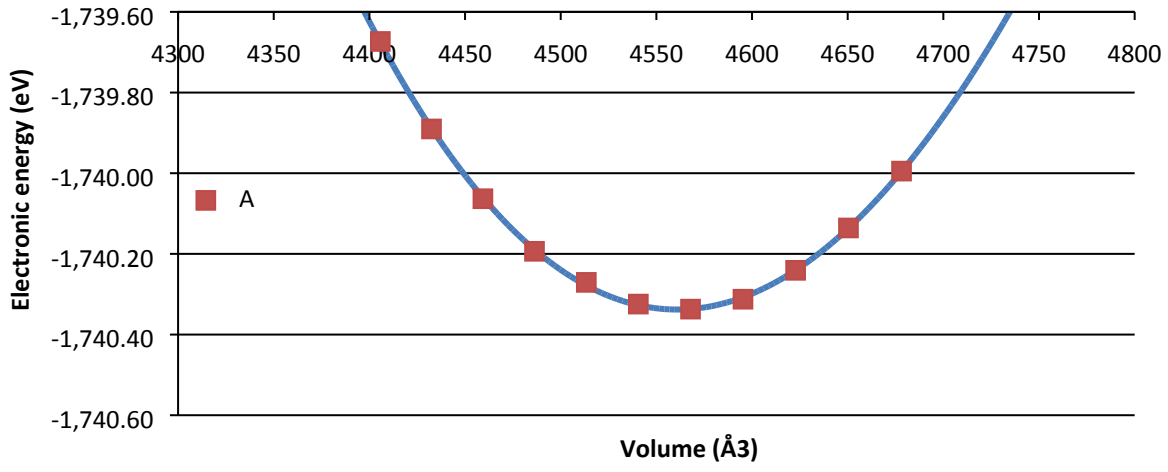
We have computed both moduli ($K_R$ and $G_R$) for all structures along the reaction NEB pathways. For transition state structures, the imaginary frequency of the Hessian related to the transition state will disturb the pseudo-inverse calculation of the Hessian in the relaxed-ion elasticity tensor, so it is not permitted to use the harmonic approach in transition state structures. Moreover, most structures of the E pathway and F pathway show numerical instability in the computation of the relaxed-ion tensor. The main manuscript therefore reports only start point and end point structures of the pathways, for which we have obtained numerically accurate relaxed-ion C tensor.

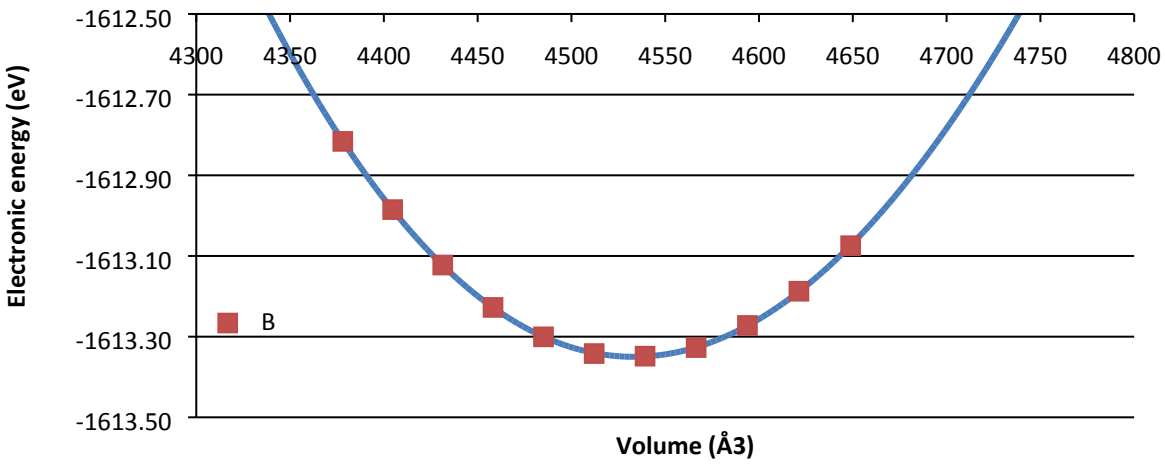
## Bulk moduli for structures A, B, C, D, E and F

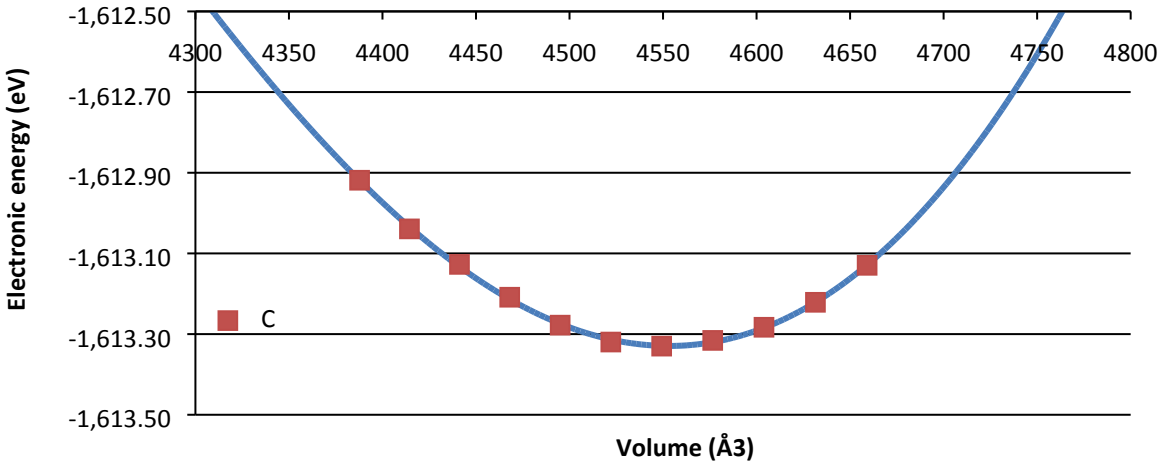
To obtain the unit cell parameters of the periodic models we have to determine their energetically most optimum volume. For the six structures A-F the unit cell parameters were first scaled (e.g. typically 99%, 99.2%, 99.4%, 99.6%, 99.8%, 100.0%, 100.2%, 100.4%, 100.6%, 100.8%, 101.0%) and a constant volume relaxation was performed. The volume dependence of the obtained energies (E(V)) was obtained by fitting the data to the Birch-Murnaghan[3] equation of state;

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^3 B_0' + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^2\left[6 - 4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]\right\}$$

With respectively the equilibrium volume $V_0$, the bulk modulus $B_0 = -V\left(\frac{\partial P}{\partial V}\right)_{P=0}$, and its derivative to the pressure $B_0' = \left(\frac{\partial B}{\partial P}\right)_{P=0}$. The Birch-Murnaghan fits for the structures A-F are given below (the obtained parameters $B_0$, $V_0$ are in **Table 1**, manuscript).




-1612.50
-1612.70
-1612.90
-1613.10
-1613.30
-1613.50
4300
4350
4400
4450
4500
4550
4600
4650
4700
4750
4800
Electronic energy (eV)
B
Volume (Å3)


-1,612.50
-1,612.70
-1,612.90
-1,613.10
-1,613.30
-1,613.50
4300
4350
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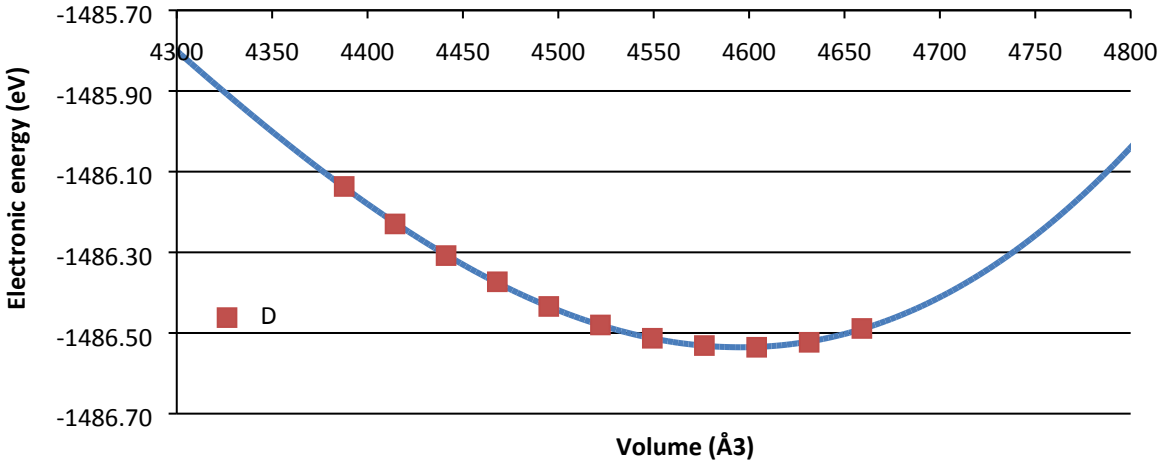
4500
4550
4600
4650
4700
4750
4800
Electronic energy (eV)
C
Volume (Å3)


-1485.70
-1485.90
-1486.10
-1486.30
-1486.50
-1486.70
4300
4350
4400
4450
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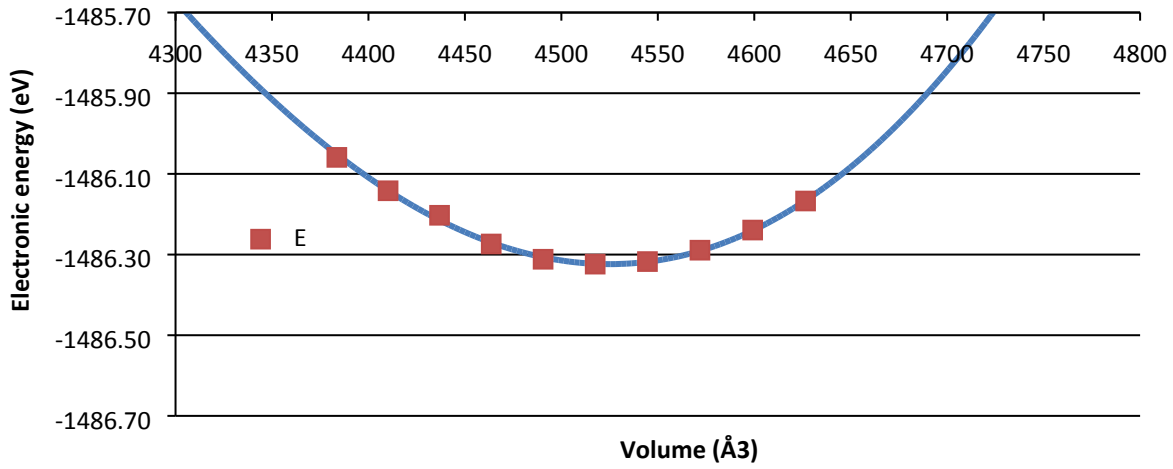
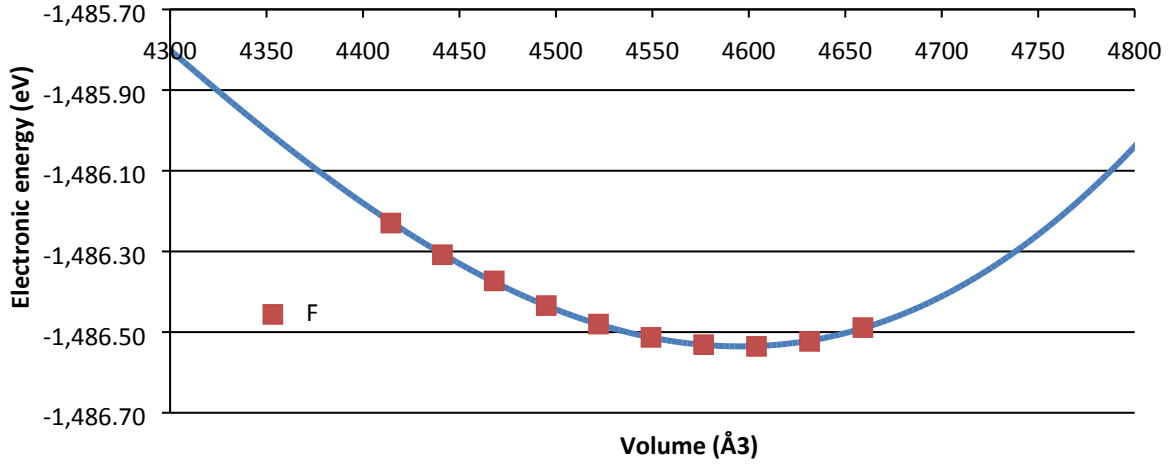
4800
Electronic energy (eV)
D
Volume (Å3)




Based on the Birch-Murnaghan fit, a new geometry was proposed, with a volume laying exactly in the minimum of the fit. Subsequently, we optimized this structure with fixed volume, followed by a general cell optimization were the volume was again allowed to expand/contract. As such, we obtained the starting structures for normal mode calculations. Once the most stable unit cell volumes were determined, we started with the investigation of the various dehydroxylation reaction pathways.

## 2.2 Implementation of elastic constants within the partition function

**Free energy associated with unit cell.** The bulk modulus can be used to write an expansion of the energy about the minimum energy point up to second order in the volume deviation V-$V_0$,

$$E = \frac{1}{2}\left(\frac{\partial^2 E}{\partial V^2}\right)_0 (V - V_0)^2 = \frac{1}{2}\frac{B}{V_0}(V - V_0)^2$$

Fluctuations in volume caused by framework flexibility will therefore contribute to the partition function. This volume contribution $Q_{vol}$ may be calculated by integrating the Boltzmann factor, where $V_0$ is used as a reference volume ($dV/V_0$):

$$Q_{\mathrm{vol}} = \int \frac{dV}{V_0}\, e^{-\frac{1}{2k_BT}\frac{B}{V_0}(V-V_0)^2} = \sqrt{\frac{2\pi k_B T}{BV_0}}$$

We find that the corresponding free energy $F_{vol}$, caused by volume fluctuations, is equal to

$$F_{\mathrm{vol}} = -k_B T \ln \sqrt{\frac{2\pi k_B T}{BV_0}}$$

Flexible materials are characterized by a small bulk modulus, such that $Q_{vol}$ is large, and the free energy might be reduced considerable by the free energy $F_{vol}$. This corresponds to the idea that a flexible material can explore more states because of the volume fluctuations, thus lowering its free energy due to entropy. This effect becomes more important at higher temperature, as the sampling of volume fluctuations becomes then more efficient. For stiff materials, the contribution $F_{vol}$ is small. E.g. for bcc iron with B approximately equal to 100 GPa and a volume of 5867 Å$^3$ for 1000 Fe atoms, $F_{vol}$ is approximately only 12.5 J/mol at 300 K.

**Extensivity of the free energy.** The volume free energy $F_{vol}$ per unit cell depends on the number of unit cells considered. Indeed, for $n$ unit cells taking up a volume $nV_0$ shows, $F_{vol}$ appears to be non-extensive,

$$F_{\mathrm{vol}}^{n\ \mathrm{cells}} = \frac{1}{\sqrt{n}} F_{\mathrm{vol}}^{1\ \mathrm{cell}}$$

In the limit of a large crystal, this elastic contribution to F will become negligible. This picture would be correct if the material were to stretch uniformly over all unit cells. In reality, neighboring unit cells do interact with eacht other, but they do not have to be identical copies at all times. (Volume-dependent) phon modes allow different behavior in neighboring cells. In the extreme view point, each unit cell behaves independently, such that

$$Q_{\mathrm{vol}}^{n\ \mathrm{cells}} = \left(Q_{\mathrm{vol}}^{1\ \mathrm{cell}}\right)^n$$

and the volume free energy $F_{vol}$ per unit cell only depends on $V_0$, not on n. The volume $V_0$ is then that of the cell (unit cell or supercell) where volume correlation between neighboring cells is negligible. In this work, a single UiO unit cell is approximately 4500 Å$^3$, which is already quite large, so $V_0$ is taken to be that of a single unit cell.

## 3 Comparison of the six periodic models based on (free) energy differences

**Table S.1**: Average free energy difference ΔG for the removal of a terephthalate linker (per unit cell) at different temperatures (130, 220, 320 and 450 ºC) with respect to the reference structure **A**, at a pressure of 1 bar for terephthalic acid (TA) treated in gas phase. $\Delta G = 1/x[G + x\ G_{TA} - G_A\ ]$ with x = number of removed linkers per unit cell. Unit cell consisting of two bricks. The results were obtained in a periodic calculation with the PBE-D3(BJ) functional, employing an energy cutoff of 600 eV. Also the electronic removal energy is tabulated.

| | $\Delta E_{elec}$ (kJ/mol) | $\Delta G_{130}$ *(kJ/mol)* | $\Delta G_{220}$ *(kJ/mol)* | $\Delta G_{320}$ *(kJ/mol)* | $\Delta G_{450}$ *(kJ/mol)* |
|---|---|---|---|---|---|
| **defectless structure (x=0)** | | | | | |
| A. $<Zr_6O_4(OH)_4(RCOO)_{12}>_2$ $\{12^{12}, 12^{12}\}$ | | - | - | - | - |
| **1 missing linker (x=1)** | | | | | |
| **B.** $<Zr_6O_4(OH)_4(RCOO)_{12}>$ $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $\{12^{10}, 10^{12}\}$ | 379.4 | 267.4 | 241.5 | 213.0 | 176.3 |
| **C.** $<Zr_6O_5(OH)_3(RCOO)_{11}>$ $<Zr_6O_5(OH)_3(RCOO)_{11}>$ $\{11^{11}, 11^{11}\}$ | 382.9 | 274.7 | 250.1 | 222.9 | 188.0 |
| **2 missing linkers (x=2)** | | | | | |
| **D.** $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $\{10^{10}, 10^{10}\}$ | 370.9 | 257.9 | 231.9 | 203.2 | 166.2 |
| **E.** $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $\{10^{10}, 10^{10}\}$ | 383.9 | 277.1 | 252.8 | 226.1 | 191.9 |
| **F.** $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $<Zr_6O_6(OH)_2(RCOO)_{10}>$ $\{10^{10}, 10^{10}\}$ | 368.4 | 261.2 | 236.9 | 210.2 | 175.9 |

# 4 Study of reaction pathways

## 4.1 Investigated reaction pathways

Several intermediate NEBs were constructed to determine minimum energy pathways for 9 water removal reactions and 3 oxygen transfer reactions (**Table S.1**).

**Table S.1**: different investigated water removal and oxygen transfer reactions

| | Unit cell – formula | Brick 1 | Brick 2 | Investigated $H_2O$ removals | Investigated O-transfer reactions |
|---|---|---|---|---|---|
| | **No missing linkers perfect coordination** | | | | |
| A | $<Zr_6O_4(OH)_4(RCOO)_{12}>_2$ | $[Zr_6O_4(OH)_4]^{12+}$ | $[Zr_6O_4(OH)_4]^{12+}$ | **2** | **1** |
| | **1 missing linker** | | | | |
| B | $<Zr_6O_4(OH)_4(RCOO)_{12}>$<br>$<Zr_6O_6(OH)_2(RCOO)_{10}>$ | $[Zr_6O_4(OH)_4]^{12+}$ | $[Zr_6O_6(OH)_2]^{10+}$ | **3** | **2 (for brick 2 and brick 1)** |
| C | $<Zr_6O_5(OH)_3(RCOO)_{11}>$<br>$<Zr_6O_5(OH)_3(RCOO)_{11}>$ | $[Zr_6O_5(OH)_3]^{11+}$ | $[Zr_6O_5(OH)_3]^{11+}$ | **1** | 0 |
| | **2 missing linkers (different orientation of the defects)** | | | | |
| D | $<Zr_6O_6(OH)_2(RCOO)_{10}>$<br>$<Zr_6O_6(OH)_2(RCOO)_{10}>$ | $[Zr_6O_6(OH)_2]^{10+}$ | $[Zr_6O_6(OH)_2]^{10+}$ | **1** | 0 |
| E | $<Zr_6O_6(OH)_2(RCOO)_{10}>$<br>$<Zr_6O_6(OH)_2(RCOO)_{10}>$ | $[Zr_6O_6(OH)_2]^{10+}$ | $[Zr_6O_6(OH)_2]^{10+}$ | **1** | 0 |
| F | $<Zr_6O_6(OH)_2(RCOO)_{10}>$<br>$<Zr_6O_6(OH)_2(RCOO)_{10}>$ | $[Zr_6O_6(OH)_2]^{10+}$ | $[Zr_6O_6(OH)_2]^{10+}$ | **1** | 0 |
| | | | | | |

All investigated reaction pathways are indicated in **Figures S.3** and **S.4**.

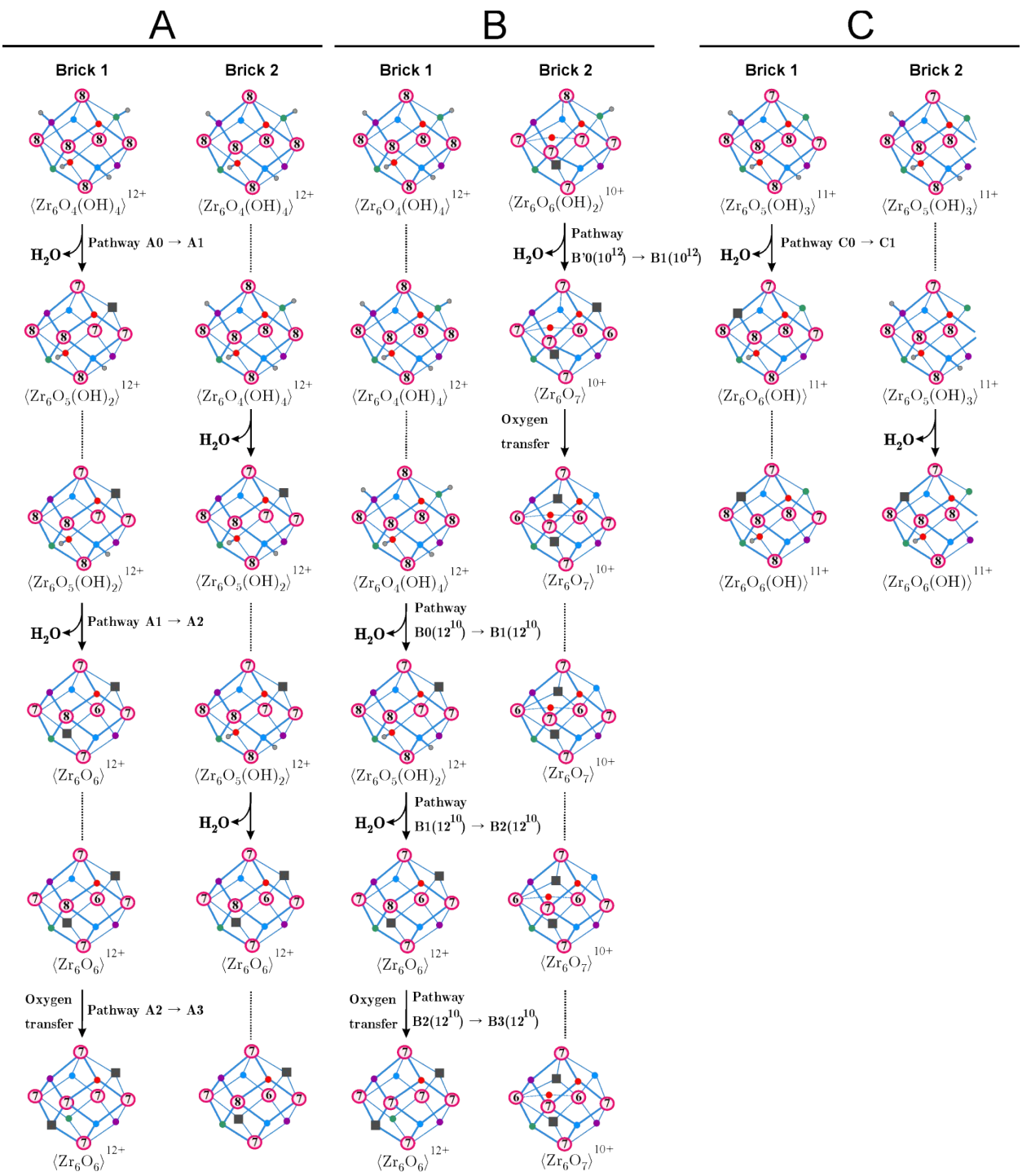



**Figure S.3** Investigated pathways for structures A, B and C

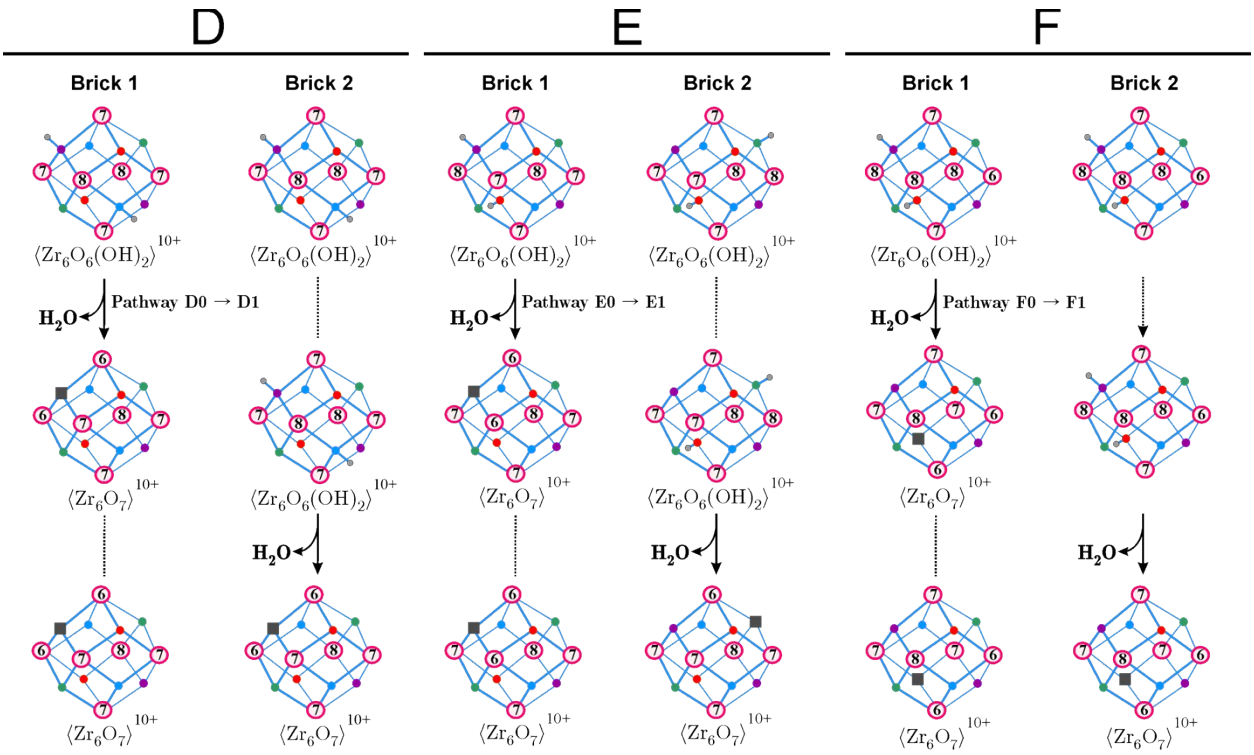
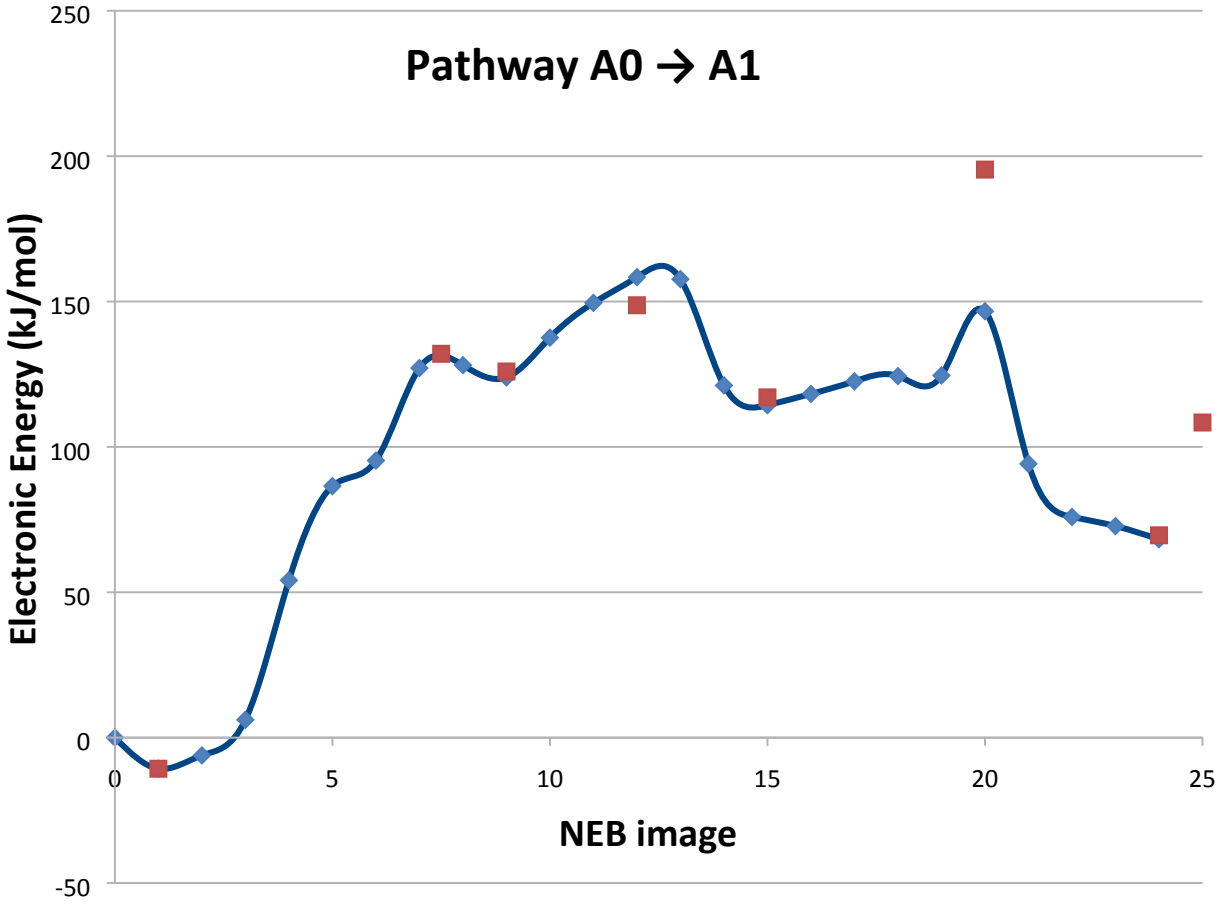


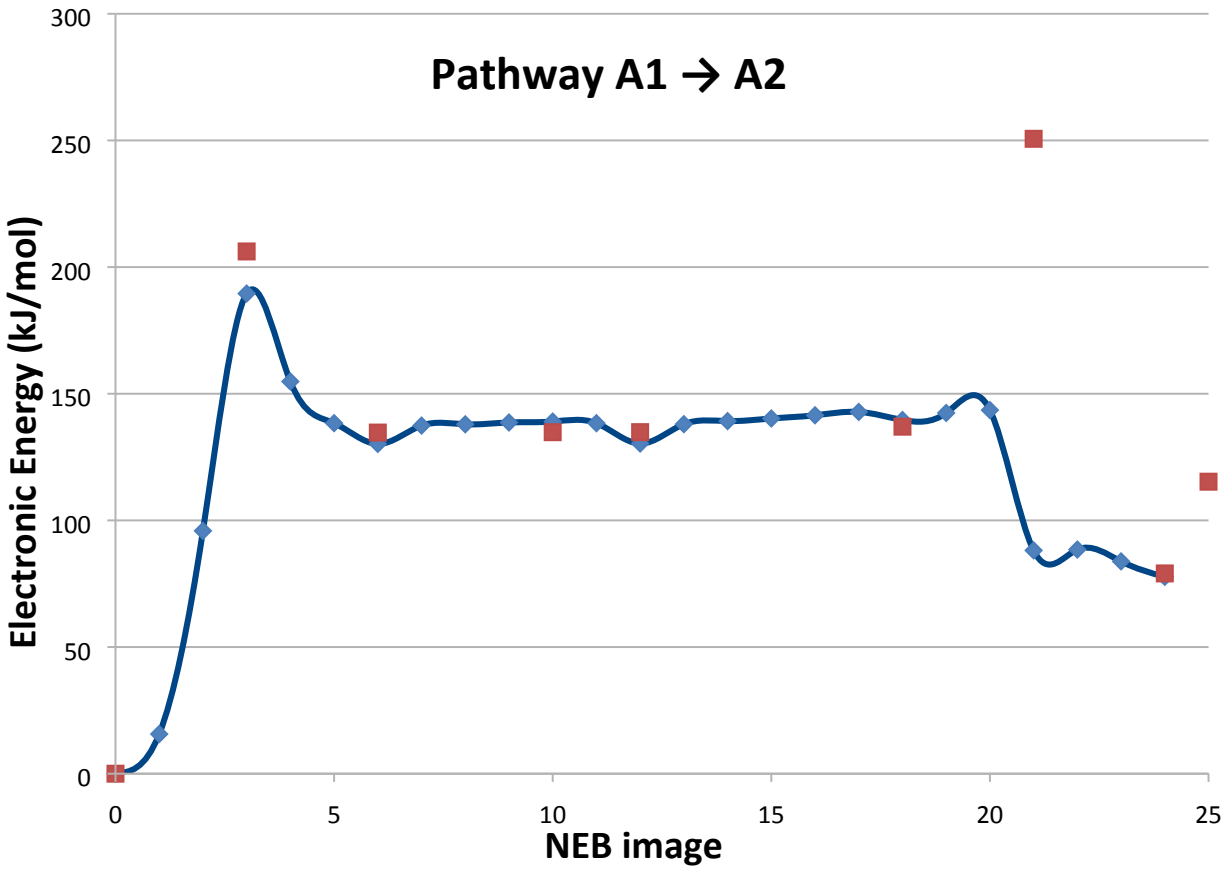

**Figure S.4** Investigated pathways for structures D, E and F

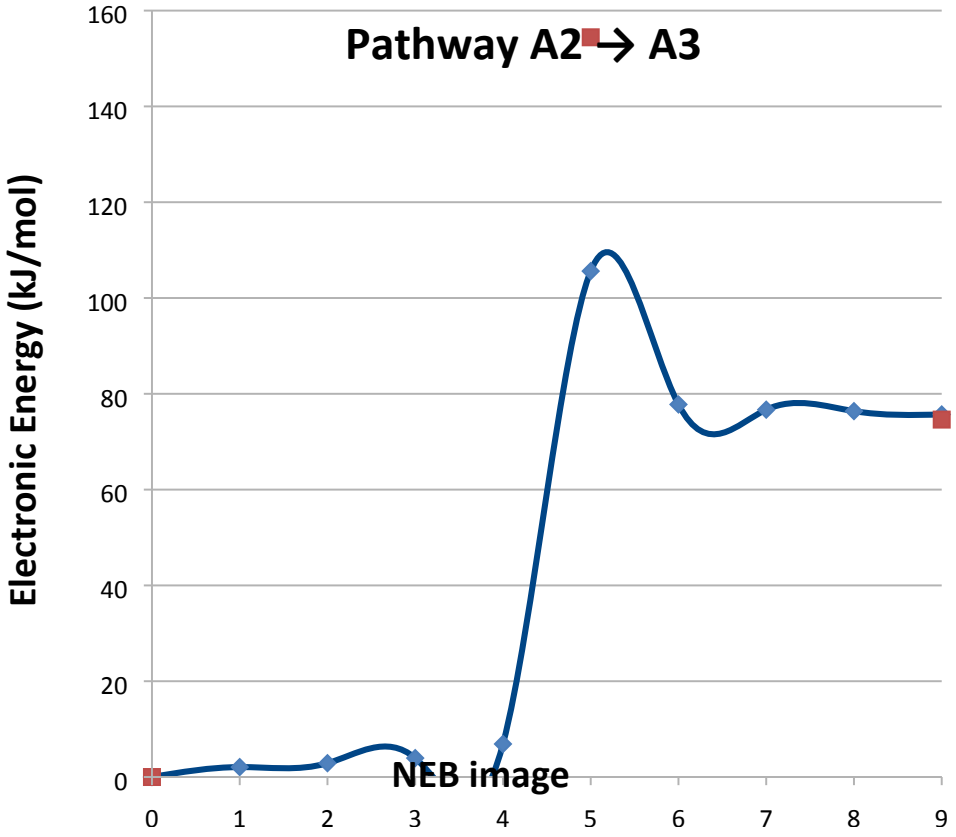
## 4.2 Energetic profiles for the NEB-simulations

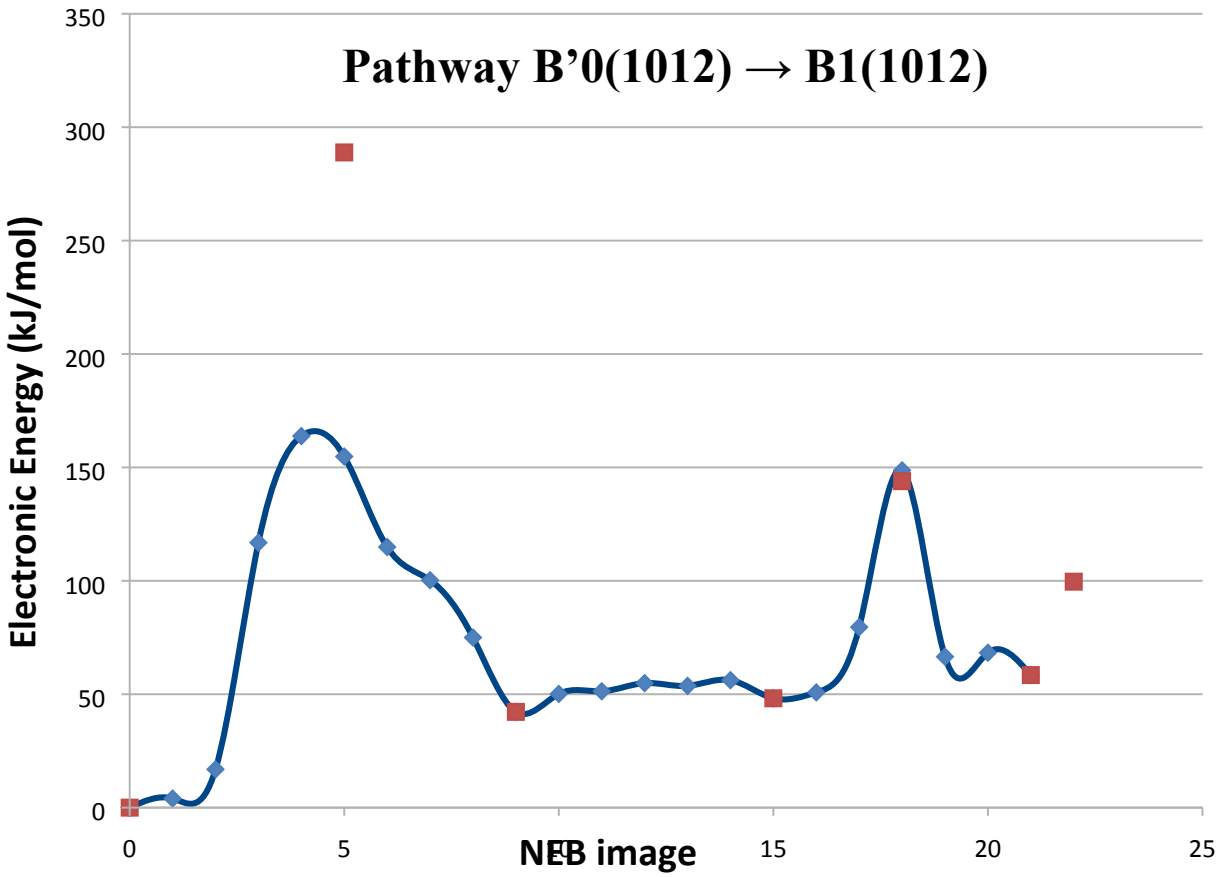
The energetic profiles are given below and were obtained by linking several NEB simulations along the reaction path. Refinements on local reactants and transition states along this path were then performed (points in red), followed by a full normal mode calculations.

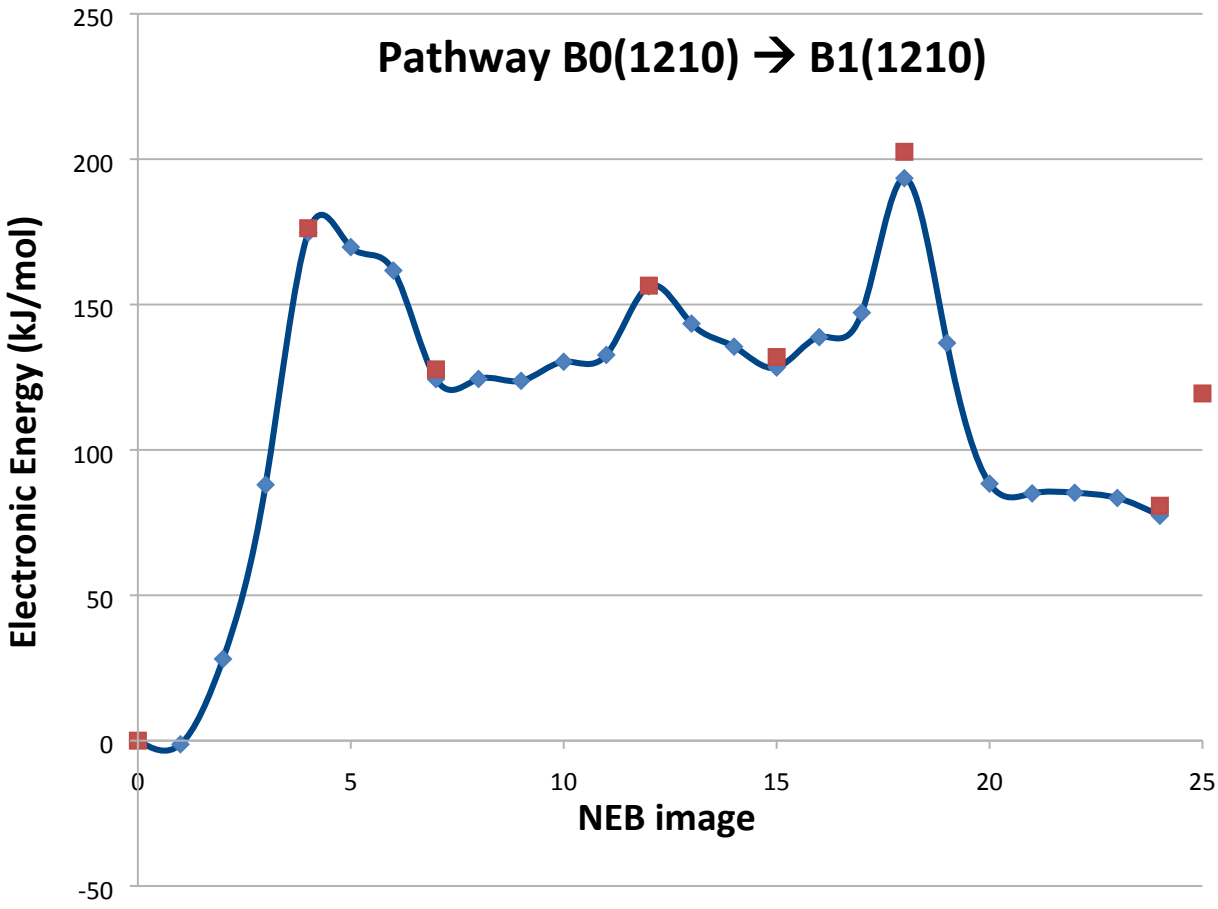
For **Pathways A0 → A1, A1 → A2, A2 → A3, B0($12^{10}$) → B1($12^{10}$), B1($12^{10}$) → B2($12^{10}$), B2($12^{10}$) → B3($12^{10}$) , D0 → D1, E0 → E1, F0 → F1** the normal mode analysis of the product structure (in which water was formed) contained still 1 imaginary mode.

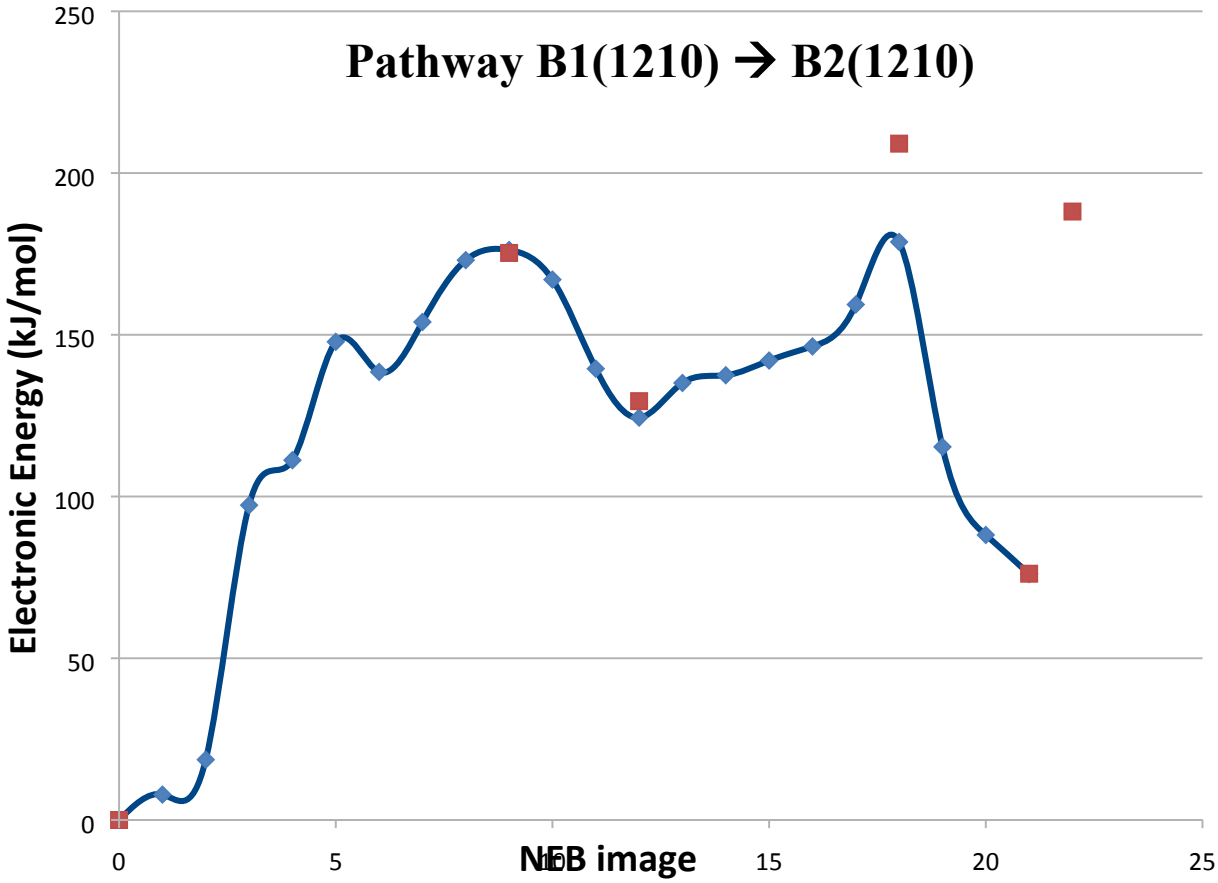

Pathway A0 → A1
Electronic Energy (kJ/mol)
250
200
150
100
50
0
-50
0
5
10
15
20
25
NEB image

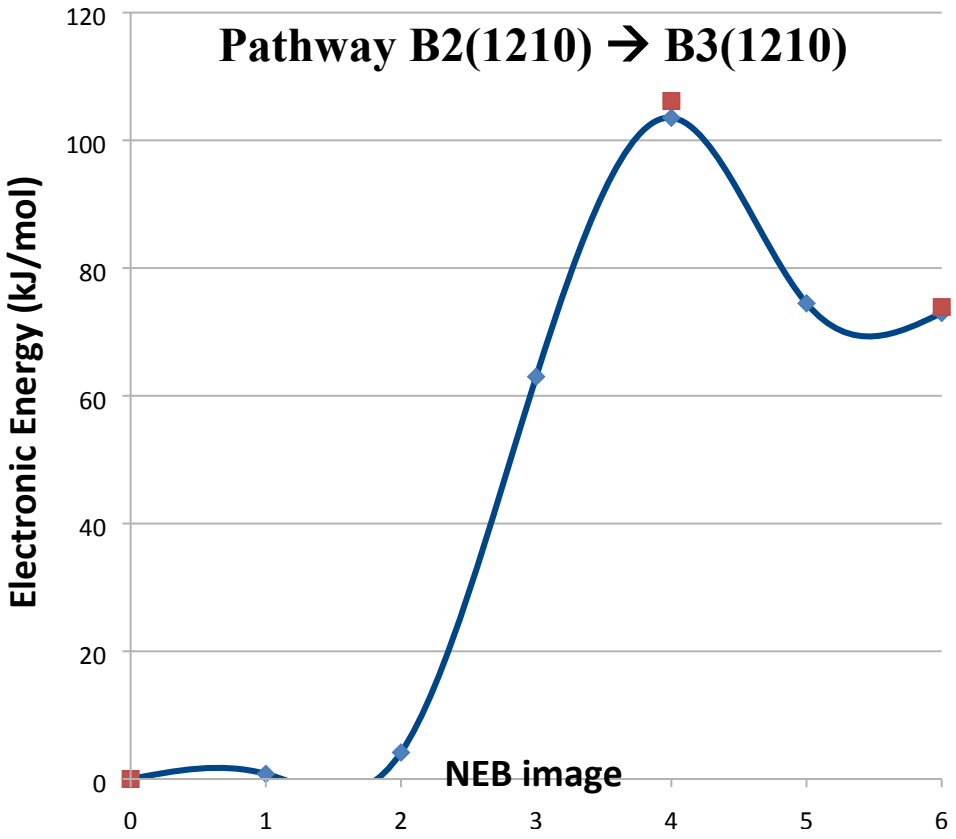

Pathway A1 → A2
Electronic Energy (kJ/mol)
300
250
200
150
100
50
0
0
5
10
15
20
25
NEB image

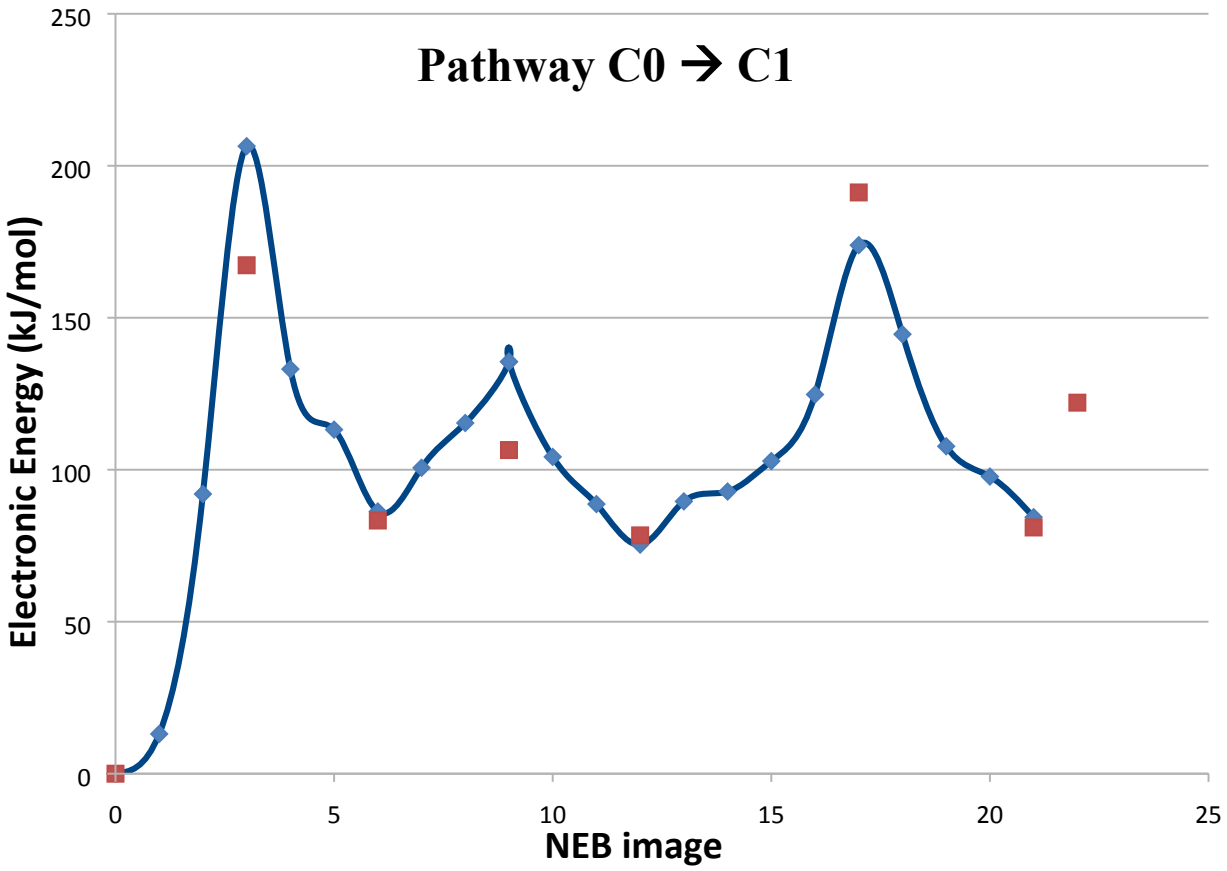

Pathway A2 → A3
Electronic Energy (kJ/mol)
160
140
120
100
80
60
40
20
0
0
1
2
3
4
5
6
7
8
9
NEB image

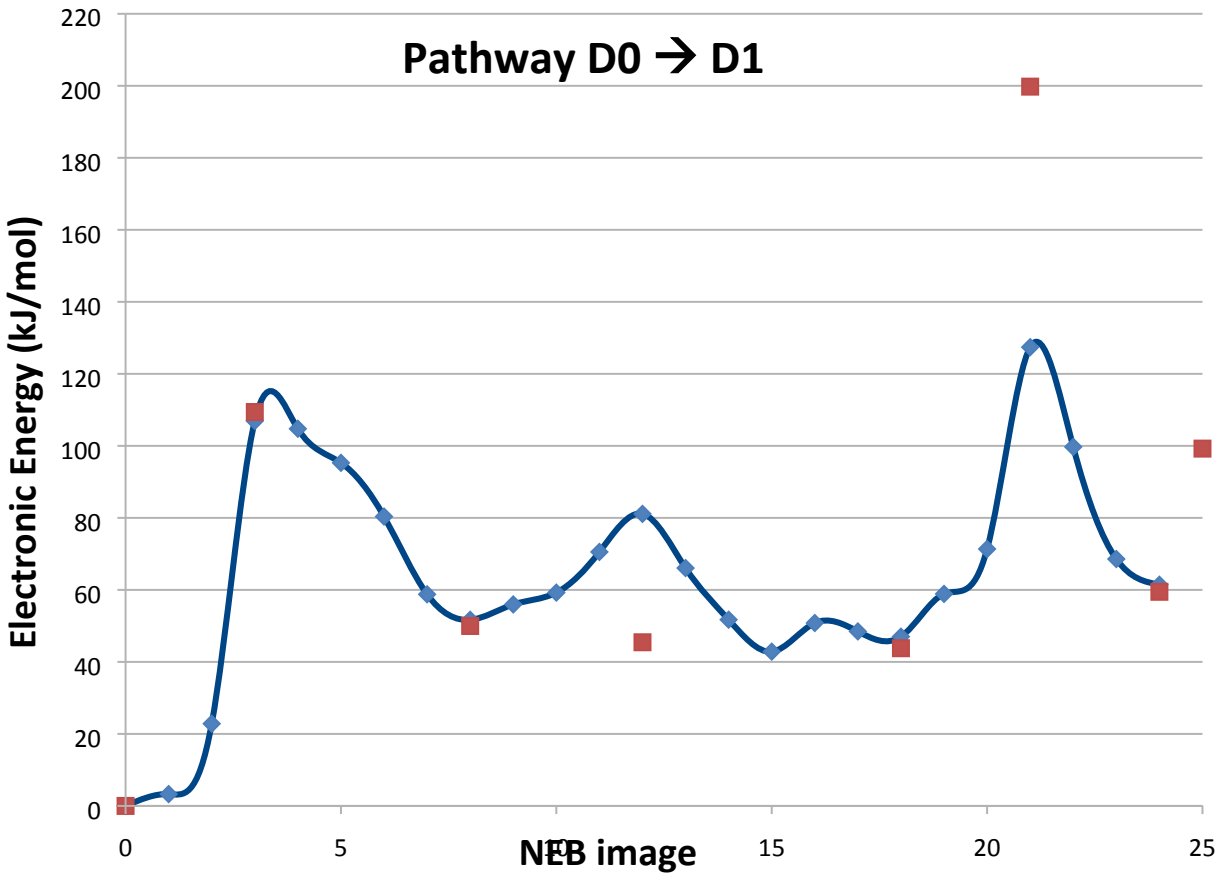

Pathway B'0(1012) → B1(1012)
Electronic Energy (kJ/mol)
350
300
250
200
150
100
50
0
0
5
15
20
25
NEB image

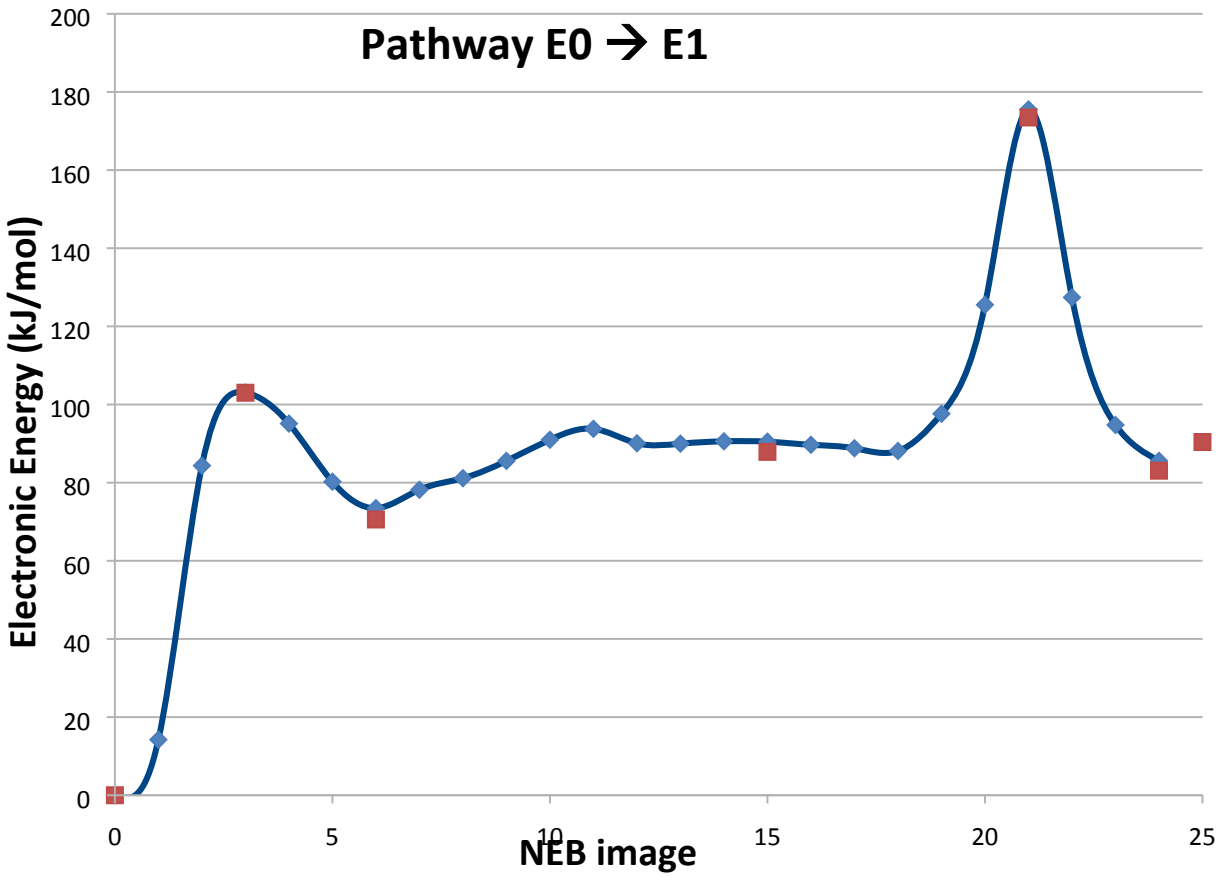

Pathway B0(1210) → B1(1210)
Electronic Energy (kJ/mol)
250
200
150
100
50
0
-50
0
5
10
15
20
25
NEB image

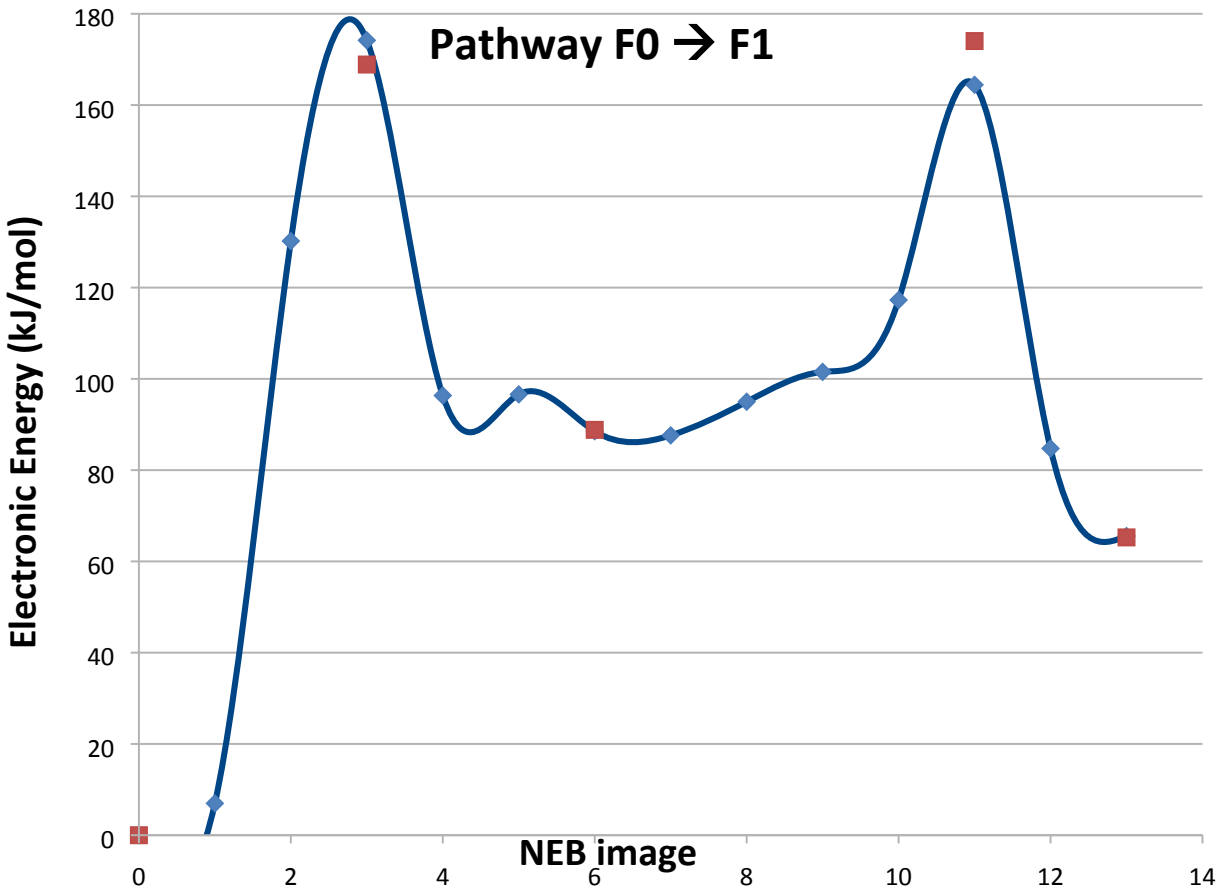

Pathway B1(1210) → B2(1210)
Electronic Energy (kJ/mol)
250
200
150
100
50
0
0
5
10
15
20
25
NEB image


Pathway B2(1210) → B3(1210)
Electronic Energy (kJ/mol)
120
100
80
60
40
20
0
NEB image
0
1
2
3
4
5
6


Pathway C0 → C1
Electronic Energy (kJ/mol)
250
200
150
100
50
0
0
5
10
15
20
25
NEB image

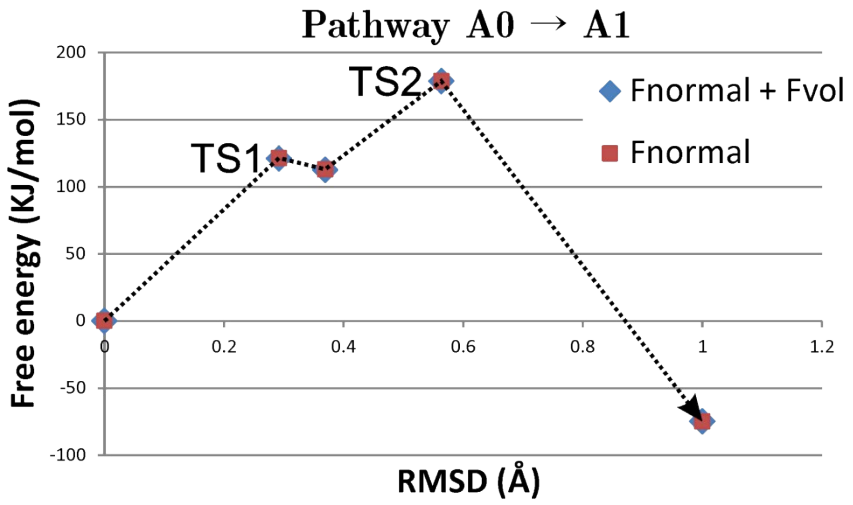

Pathway D0 → D1
Electronic Energy (kJ/mol)
220
200
180
160
140
120
100
80
60
40
20
0
0
5
15
20
25
NEB image

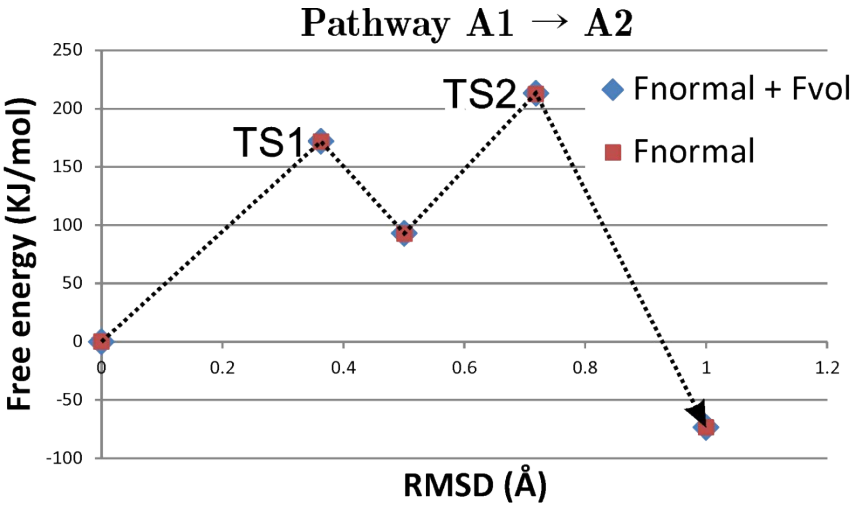

Pathway E0 → E1
Electronic Energy (kJ/mol)
200
180
160
140
120
100
80
60
40
20
0
0
5
10
15
20
25
NEB image

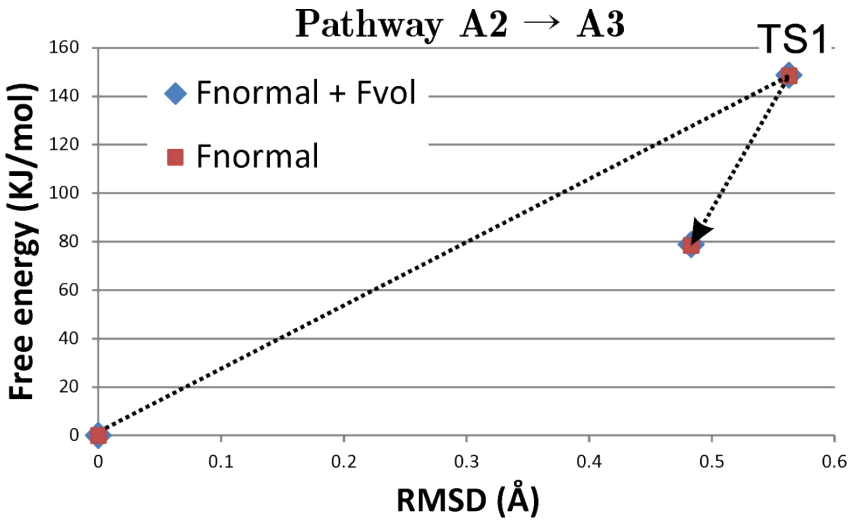



## 4.3 Free energy profiles of the modeled reaction pathways (with and without correction for elastic constants)

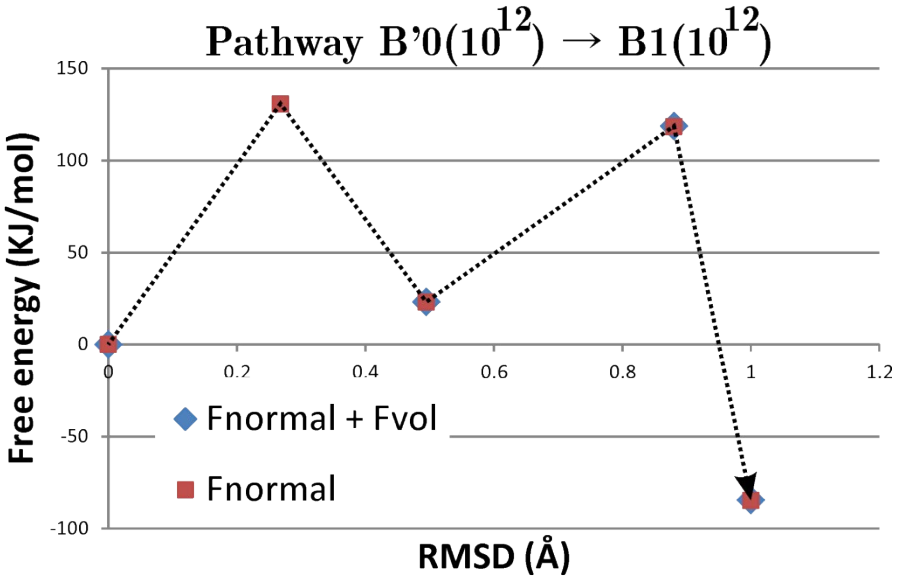
For the selected points (red squares in the section above, Energetic profiles for the NEB-simulations), a normal mode calculation was performed. Furthermore, the obtained free energies (Fnormal, see below) were then further corrected (Fnormal+Fvol, see below). This did not lead to huge differences in the free energy profiles, we observed mostly corrections of less than 1 kJ/mol at 320 °C, and in some exceptions corrections larger than 2 kJ/mol (< 6 kJ/mol). Below, the free energy profiles are given (with and without correction for the elastic constants & volume changes) with respect to the root mean square deviation (RMSD in Ångström) to the first structure (indicated by Fnormal & Fnormal+Fvol, respectivel). In the free energy profiles for the water removal pathways, water was treated in gas phase in the last step. Therefore, the RMSD for the last step was arbitrary put on 1 (or 2 in case of Pathway **D0 → D1**). Remark that in case of a transition state, the calculation of the elastic tensor is not reliable, simply because the Hessian is not positive definit. If a negative value for v1 was found, then the free energy (Fnormal + Fvol) was omitted on the plots.

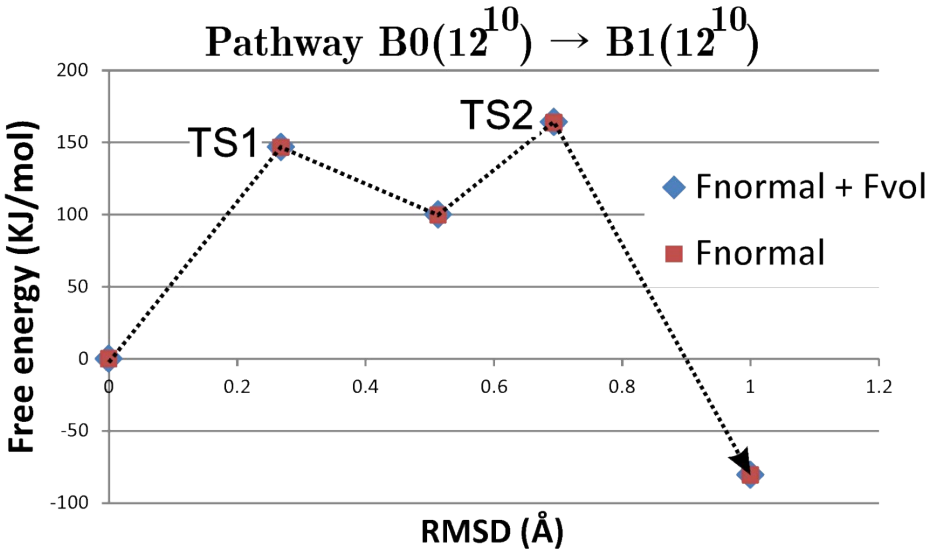

Pathway A0 → A1
Free energy (KJ/mol)
RMSD (Å)
TS1
TS2
Fnormal + Fvol
Fnormal
200
150
100
50
0
-50
-100
0
0.2
0.4
0.6
0.8
1
1.2

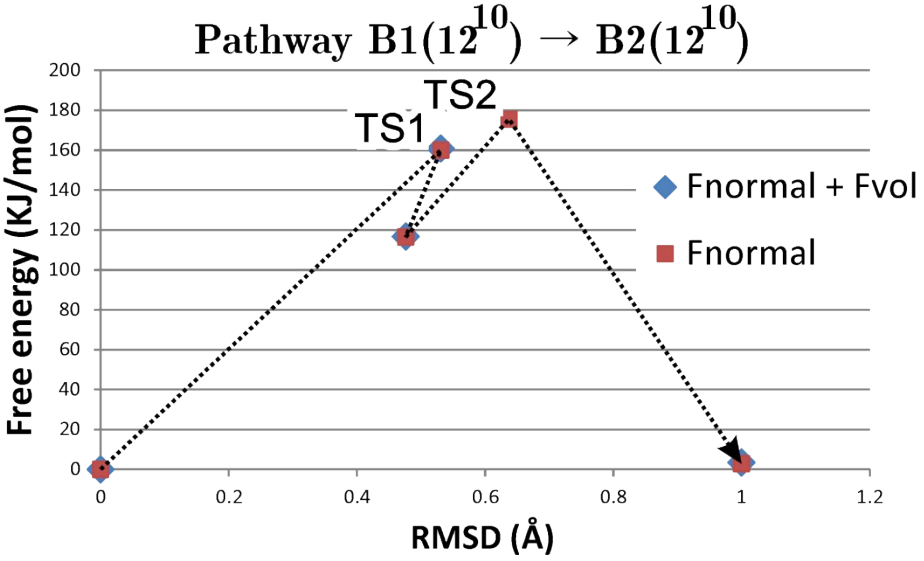

Pathway A1 → A2
Free energy (KJ/mol)
RMSD (Å)
TS1
TS2
Fnormal + Fvol
Fnormal
250
200
150
100
50
0
-50
-100
0
0.2
0.4
0.6
0.8
1
1.2

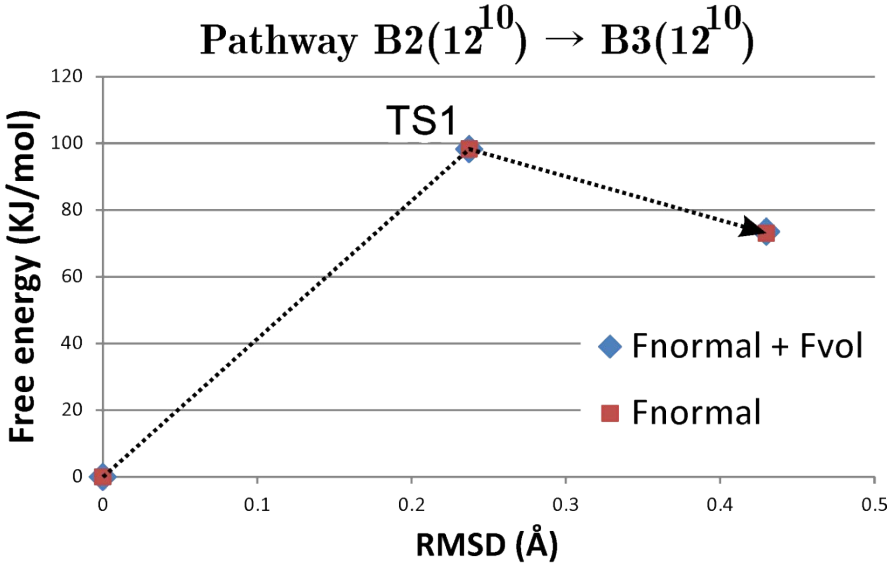

Pathway A2 → A3
Free energy (KJ/mol)
RMSD (Å)
TS1
Fnormal + Fvol
Fnormal
160
140
120
100
80
60
40
20
0
0
0.1
0.2
0.3
0.4
0.5
0.6

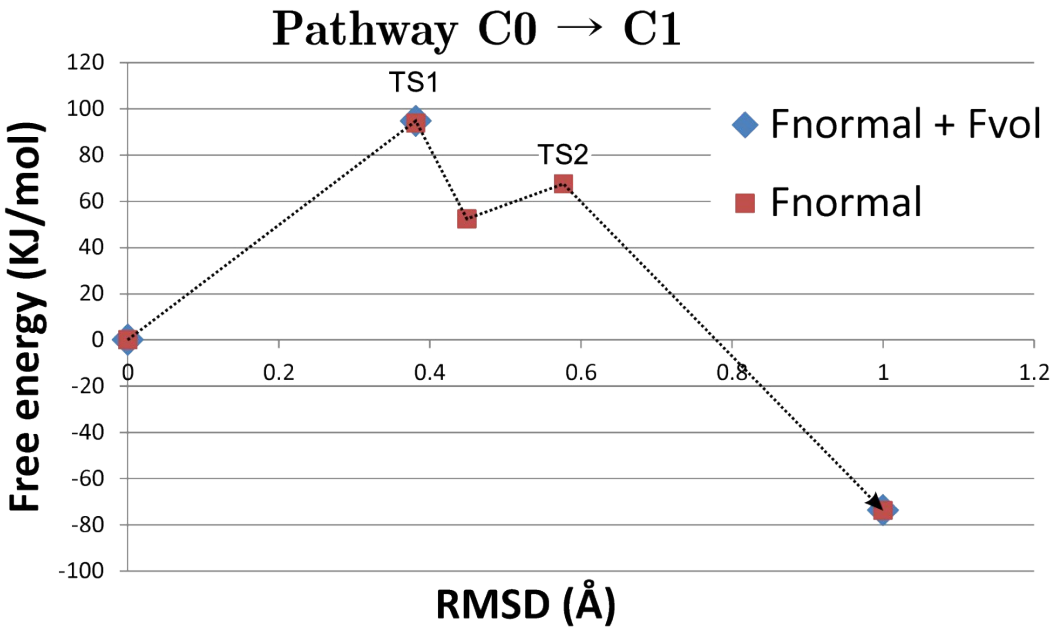
For TS1 of pathway **B0($12^{10}$) → B1($12^{10}$)**, an extra imaginary frequency was found that could not be projected out after several geometry perturbations, this frequency was replaced with an arbitrary frequency of 50 $cm^{-1}$ to get a reliable estimate for the free energy barrier.

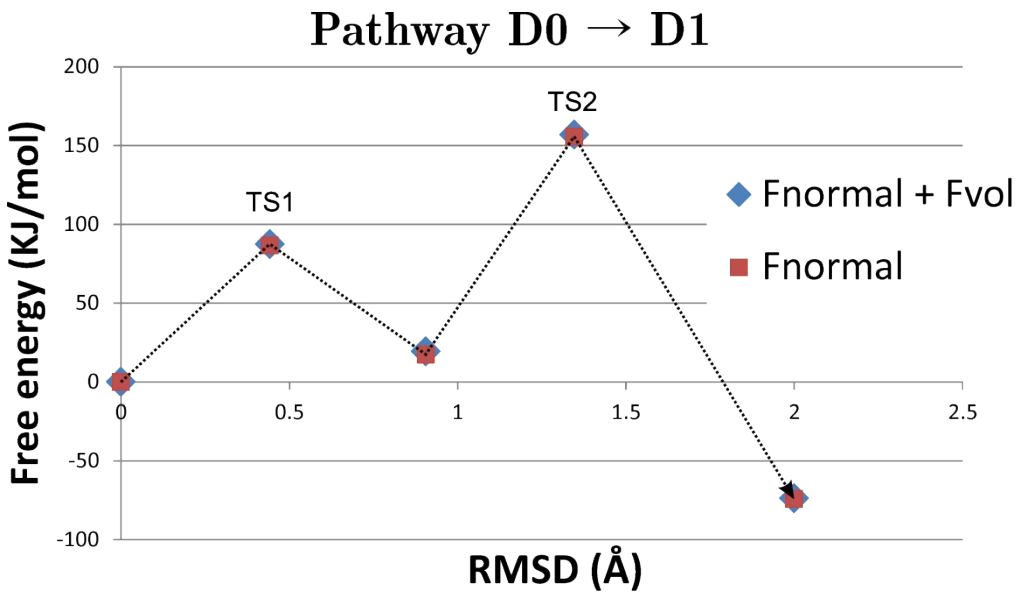


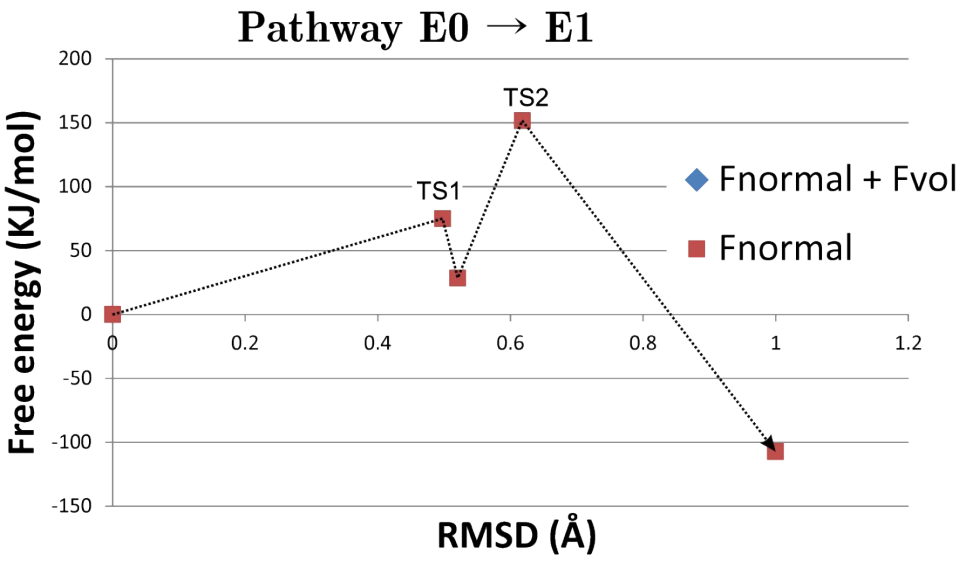



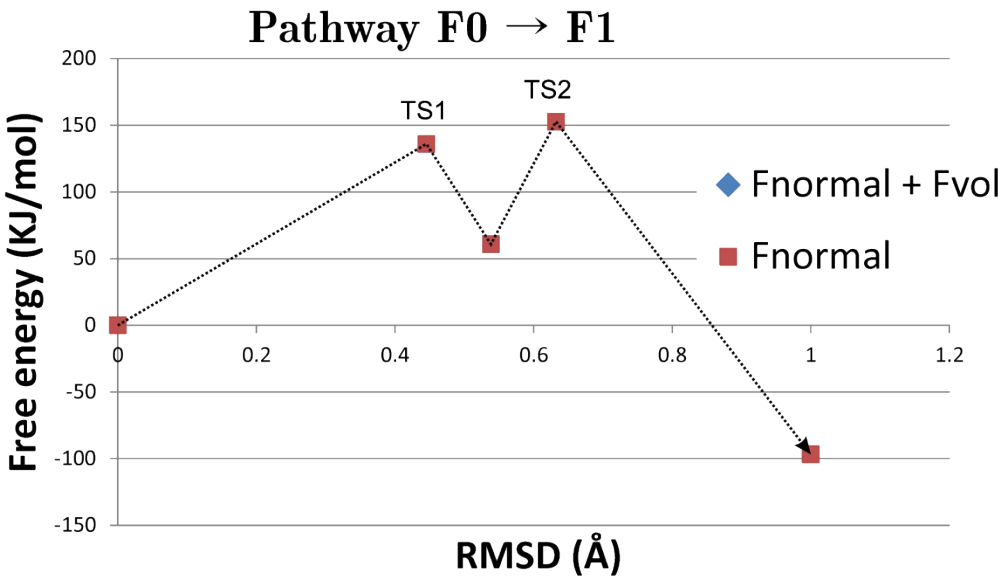

Pathway B1(12^10) → B2(12^10)
TS1
TS2
Free energy (KJ/mol)
RMSD (Å)
Fnormal + Fvol
Fnormal
0
20
40
60
80
100
120
140
160
180
200
0
0.2
0.4
0.6
0.8
1
1.2


Pathway B2(12^10) → B3(12^10)
TS1
Free energy (KJ/mol)
RMSD (Å)
Fnormal + Fvol
Fnormal
0
20
40
60
80
100
120
0
0.1
0.2
0.3
0.4
0.5

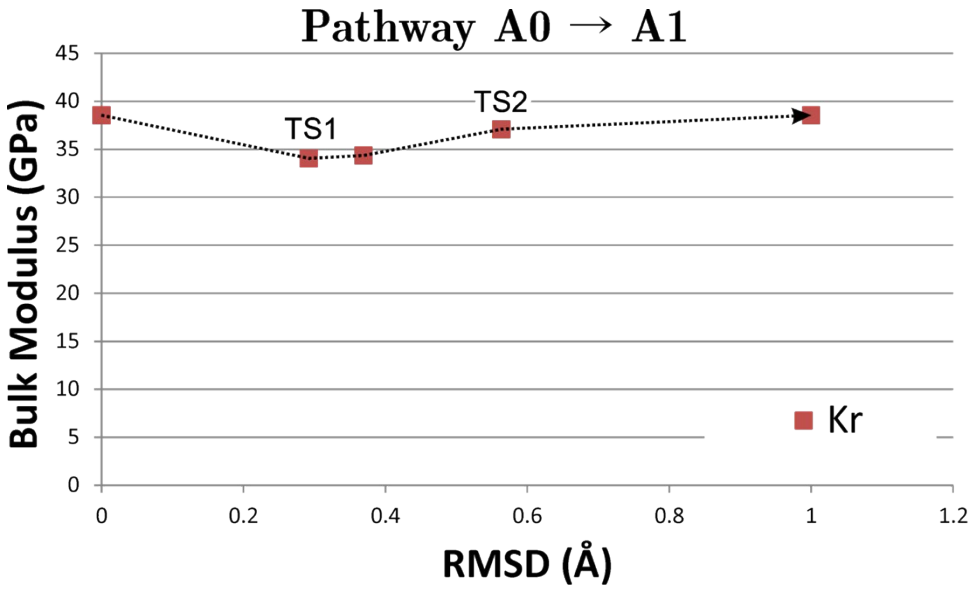

Pathway C0 → C1
TS1
TS2
Fnormal + Fvol
Fnormal
Free energy (KJ/mol)
RMSD (Å)
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
0
0.2
0.4
0.6
0.8
1
1.2

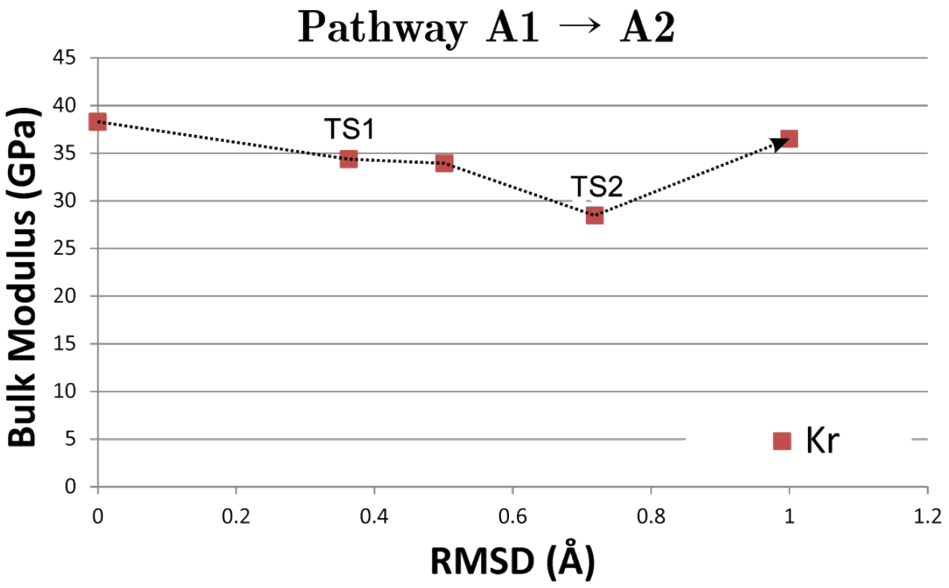

Pathway D0 → D1
TS1
TS2
Fnormal + Fvol
Fnormal
Free energy (KJ/mol)
RMSD (Å)
200
150
100
50
0
-50
-100
0
0.5
1
1.5
2
2.5

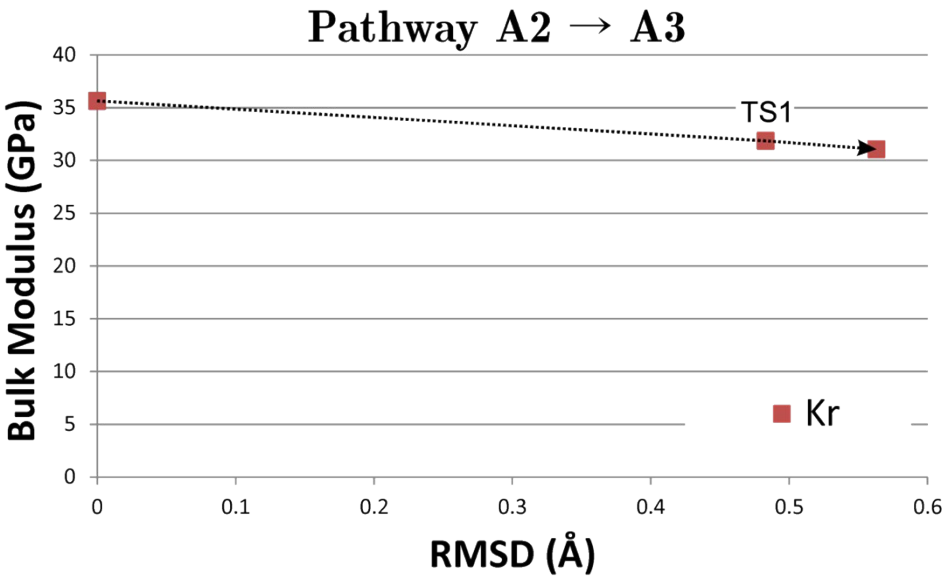


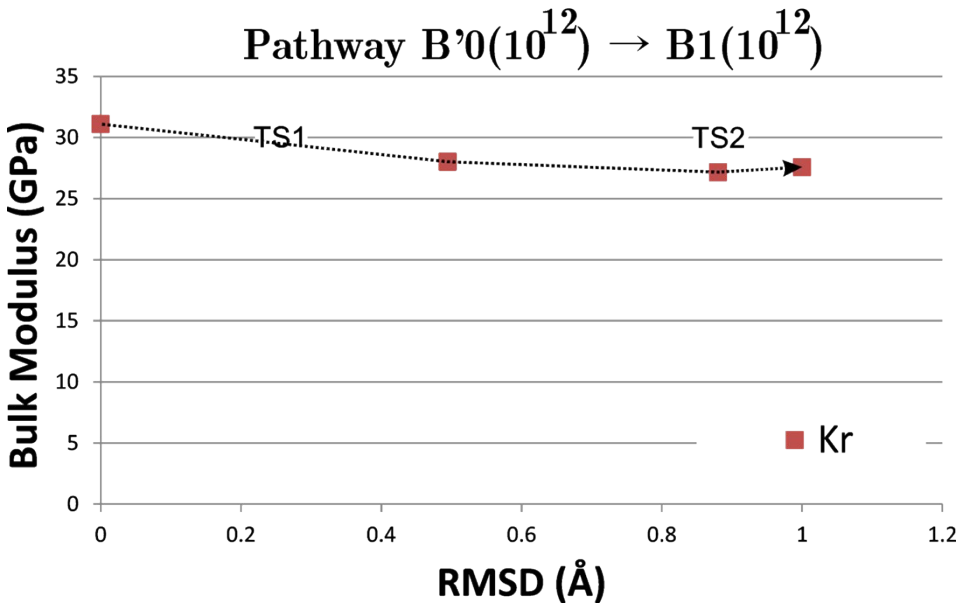



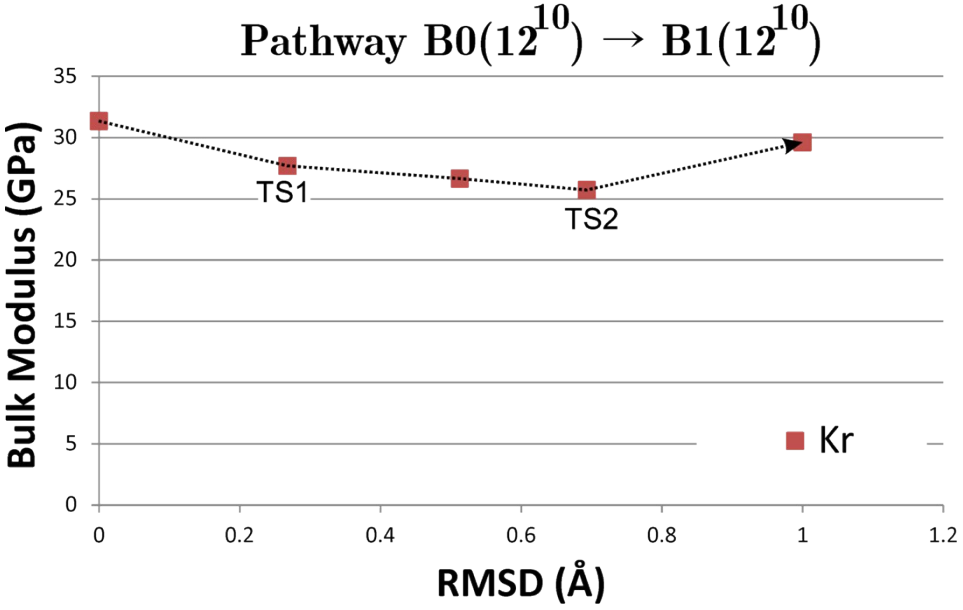

## 4.4 Bulk modules profiles of the modeled reactions

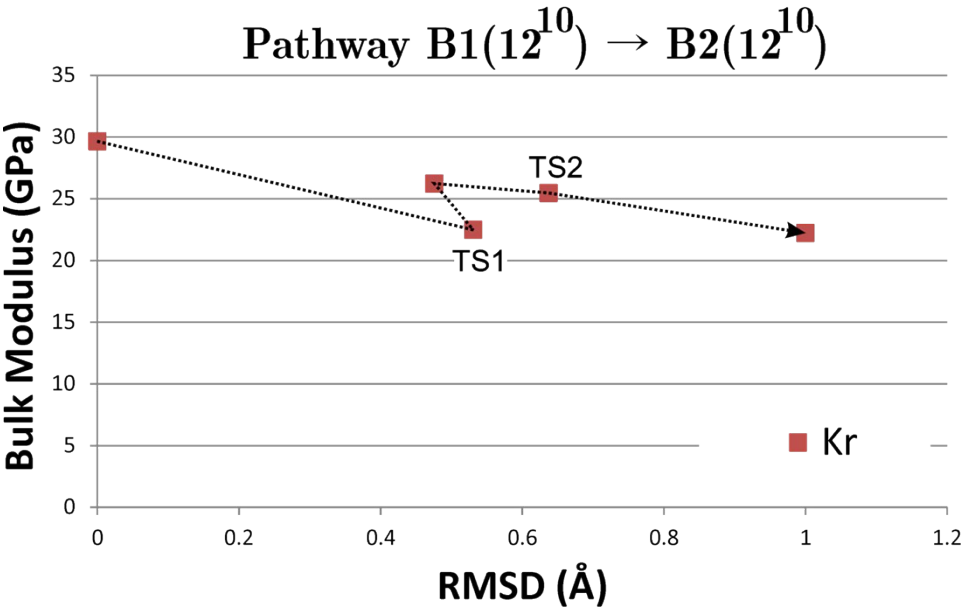

Pathway A0 → A1
Bulk Modulus (GPa)
RMSD (Å)
TS1
TS2
Kr
0
5
10
15
20
25
30
35
40
45
0
0.2
0.4
0.6
0.8
1
1.2

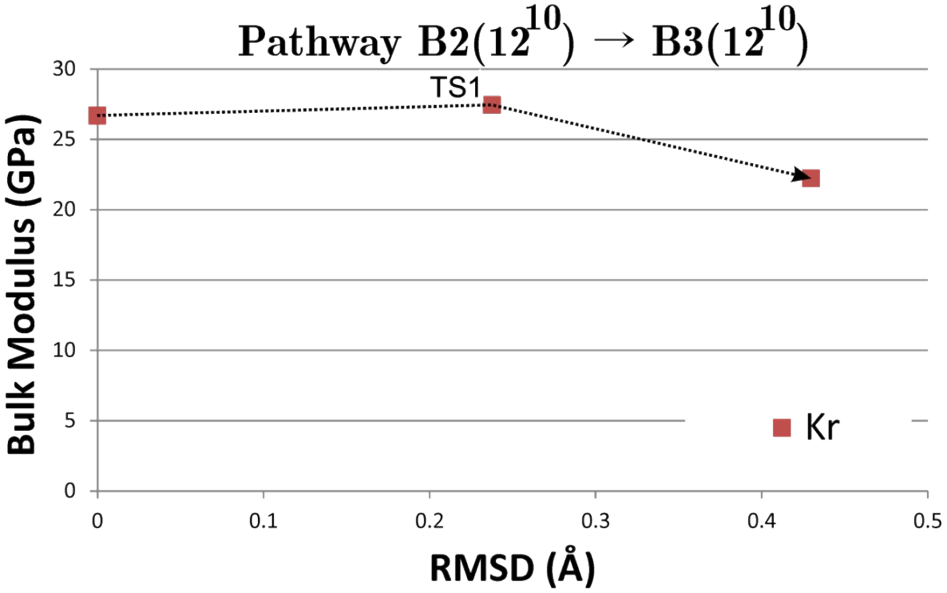

Pathway A1 → A2
Bulk Modulus (GPa)
RMSD (Å)
TS1
TS2
Kr
0
5
10
15
20
25
30
35
40
45
0
0.2
0.4
0.6
0.8
1
1.2

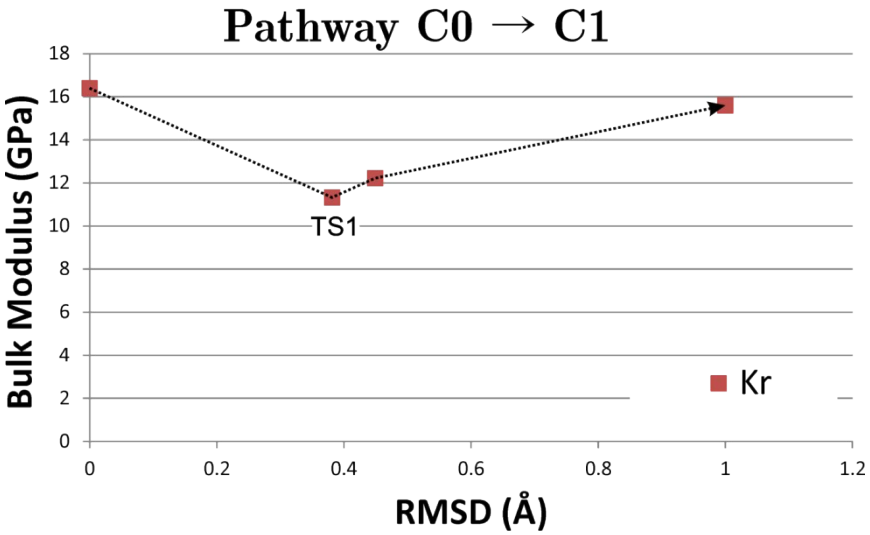

Pathway A2 → A3
Bulk Modulus (GPa)
RMSD (Å)
TS1
Kr
0
5
10
15
20
25
30
35
40
0
0.1
0.2
0.3
0.4
0.5
0.6

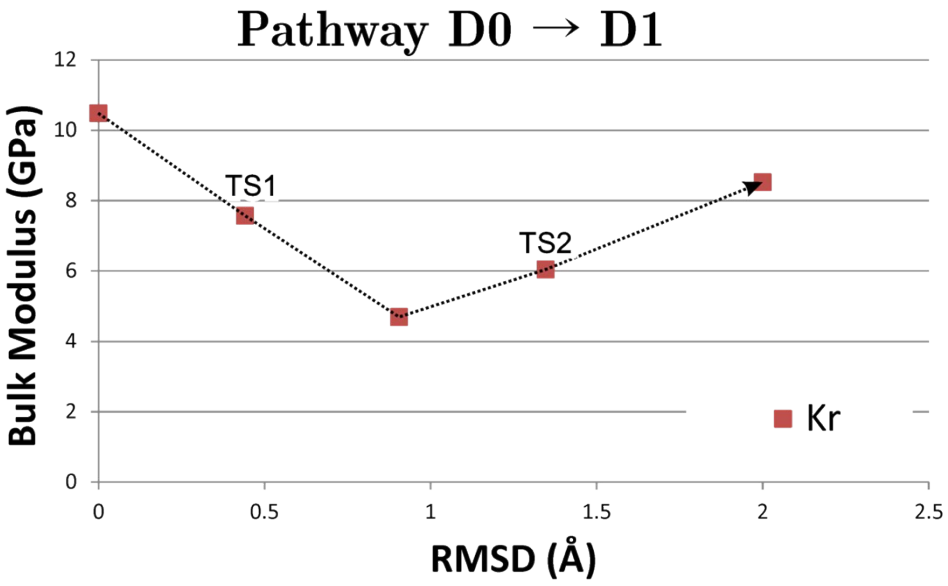

Pathway B'0(10^12) → B1(10^12)
Bulk Modulus (GPa)
RMSD (Å)
TS1
TS2
Kr
0
5
10
15
20
25
30
35
0
0.2
0.4
0.6
0.8
1
1.2

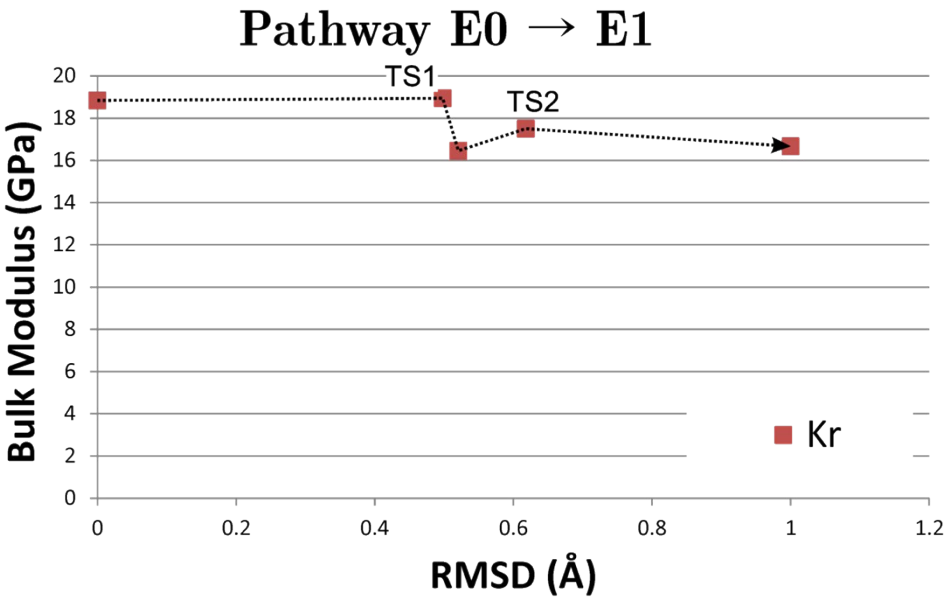

Pathway B0(12^10) → B1(12^10)
Bulk Modulus (GPa)
35
30
25
20
15
10
5
0
TS1
TS2
Kr
0
0.2
0.4
0.6
0.8
1
1.2
RMSD (Å)

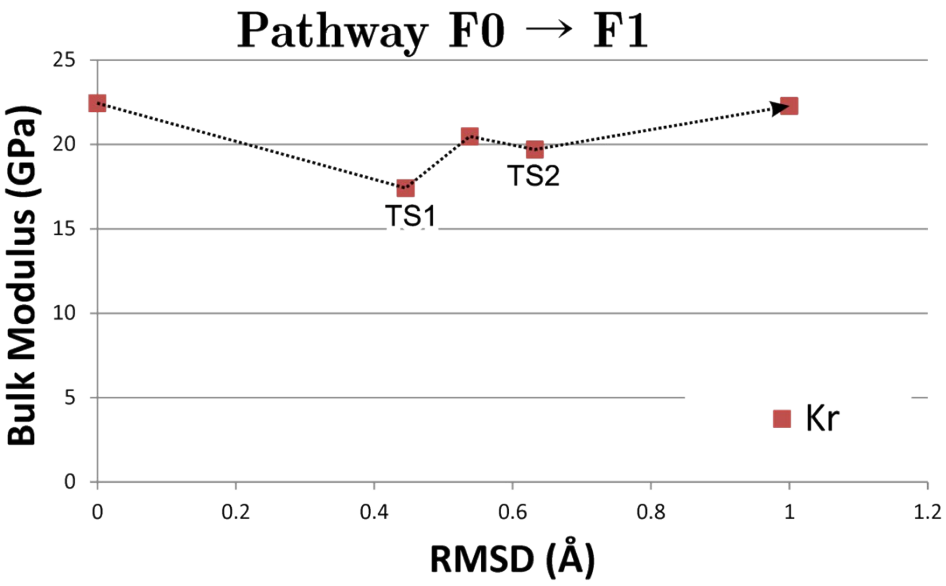

Pathway B1(12^10) → B2(12^10)
Bulk Modulus (GPa)
35
30
25
20
15
10
5
0
TS2
TS1
Kr
0
0.2
0.4
0.6
0.8
1
1.2
RMSD (Å)


Pathway B2(12^10) → B3(12^10)
TS1
Bulk Modulus (GPa)
RMSD (Å)
Kr
0
5
10
15
20
25
30
0
0.1
0.2
0.3
0.4
0.5


Pathway C0 → C1
TS1
Bulk Modulus (GPa)
RMSD (Å)
Kr
0
2
4
6
8
10
12
14
16
18
0
0.2
0.4
0.6
0.8
1
1.2


Pathway D0 → D1
Bulk Modulus (GPa)
RMSD (Å)
TS1
TS2
Kr
0
2
4
6
8
10
12
0
0.5
1
1.5
2
2.5


Pathway E0 → E1
Bulk Modulus (GPa)
RMSD (Å)
TS1
TS2
Kr
0
2
4
6
8
10
12
14
16
18
20
0
0.2
0.4
0.6
0.8
1
1.2


Pathway F0 → F1
Bulk Modulus (GPa)
25
20
15
10
5
0
0
0.2
0.4
0.6
0.8
1
1.2
RMSD (Å)
TS1
TS2
Kr

# 5 Refinement of the most stable one-linker defect structure B

In the search for the most stable one-linker defect structure B it has been observed that during the geometry optimization via static periodic calculations applying the criteria outlined in the Computational Details of the main text, an $\mu^3$oxo-oxygen is switching from the out-of-plane position to a nearby vacancy as clearly visualized in Figure 2 by comparing the bricks B0($10^{12}$) and B'0($10^{12}$). This artefact of the level of theory is removed when imposing stronger criteria on the convergence criteria and Brillouin sampling in the periodic static calculation with VASP. Following input parameters of the INCAR have been adapted:
ENCUT = 700eV (Cut-off)
ISMEAR = 0
SIGMA = 0.025
IBRION = 1
POTIM = 0.3
IVDW = 12 (D3 corrections with BJ damping)
As input in the KPOINTS file is a gamma centered mesh with a k-point grid of 2x1x2.
These settings yield an accuracy of about 1 kJ/mol on the absolute energy, which has been verified by means of a convergence test. These stronger settings have not been applied systematically to all geometry optimizations, performed in this work, due to the high number of structures and the larger computational cost.

Following E(V) curves are then obtained as displayed in Figure S.4. The volumes at the minima B'0($10^{12}$) and B0($10^{12}$) remain almost equal (V= 4575 Å$^3$).

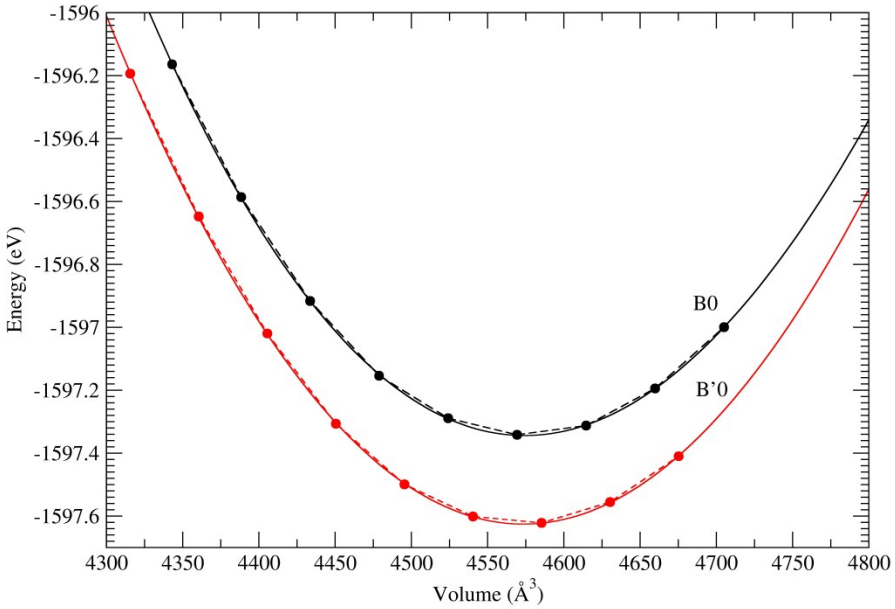



**Figure S.5**: E(V) curves for the two structures B'0($10^{12}$) and B0($10^{12}$).

The bricks corresponding with the two structures B'0($10^{12}$) and B0($10^{12}$) with the oxygen transfer are shown in Figure S.5.

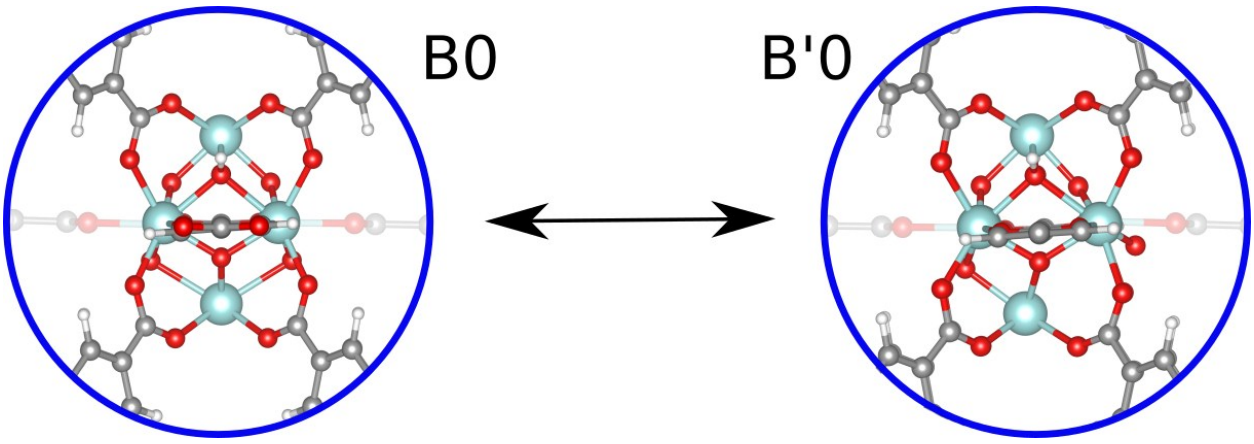



**Figure S.6**: The two structures B'0($10^{12}$) and B0($10^{12}$) with the oxygen transfer.

## 6 Free energy diagram of water coordinating to defect sites

Gibbs free energy diagram of water coordinating to defect sites, modeled on an extended cluster model of the UiO-66 at the B3LYP/[6-311++g(d,p),LanL2TZ(f)]//B3LYP/[6-31g(d),LanL2DZ] level of theory. Water molecules are approximated in gas phase; this approximation is reasonable and makes a relative comparison between the different states possible. Free energies (in kJ/mol) for the different steps in the diagram are given at different conditions of temperature and pressure.

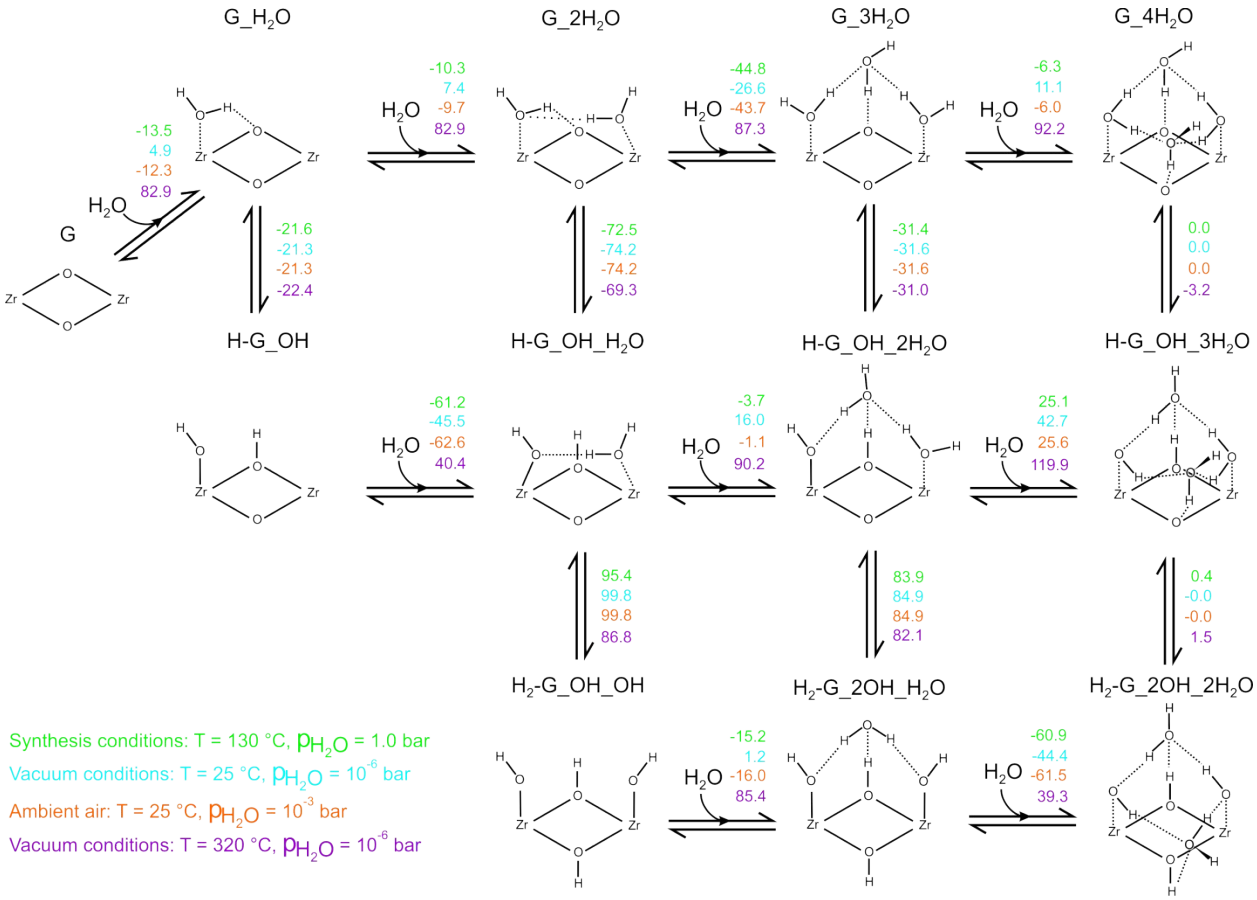



**Figure S.7:** Gibbs free energy diagram of water coordinating to defect sites, modeled on an extended cluster model of the UiO-66 at the B3LYP/[6-311++g(d,p),LanL2TZ(f)]//B3LYP/[6-31g(d),LanL2DZ] level of theory. Water molecules are approximated in gas phase; this approximation is reasonable and makes a relative comparison between the different states possible. Free energies (in kJ/mol) for the different steps in the diagram are given at different conditions of temperature and pressure.

# 7 Geometric data of the six optimized structures

In this section the cell optimized structures are given in POSCAR format.

### Structure A

```
Zr O C H
  1.00120000000000
    14.7345604804404253   -0.0027556607139181   -0.0000206312725757
     0.0047470576443588   20.8377284689999982   -0.0001311150907583
    -0.0001153399421561    0.0000832863969096   14.7347103822748302
   Zr   O    C    H
   12    64    96    56
Selective dynamics
Direct
  0.4904966294386163  0.1388844850784670  0.9800782285960664   T   T   T
  0.9901978327367814  0.6388647048840260  0.4797683796541671   T   T   T
  0.4901649218782508  0.8994350009711023  0.9799451554175916   T   T   T
  0.3706007315192990  0.0191955179994737  0.0997161875085427   T   T   T
  0.8706407145874734  0.5191127190781094  0.3599585522645311   T   T   T
  0.9903845589466529  0.3994212036894607  0.4797153551718051   T   T   T
  0.8706468568126382  0.5190757350280764  0.5994607255187687   T   T   T
  0.3706463601750099  0.0192532995429448  0.8602653377544165   T   T   T
  0.1100484474503684  0.5192084883218617  0.3599807259473896   T   T   T
  0.6100485616334319  0.0190503174034063  0.0997519702947706   T   T   T
  0.1101269504228468  0.5191644055094973  0.5993695652586349   T   T   T
  0.6100841725798452  0.0191035295701916  0.8603255226527829   T   T   T
  0.4902876789680010  0.9517008602079281  0.8450779844230608   T   T   T
  0.3223887178042437  0.1131396199801922  0.1538809680748435   T   T   T
  0.1576894002223242  0.6132242450818576  0.6539529981892651   T   T   T
  0.1251762854744971  0.5867389459504595  0.4797173976564187   T   T   T
  0.3930708083984083  0.8483155566510574  0.8889963031424154   T   T   T
  0.2255220634789638  0.0162457224530734  0.9029337520650172   T   T   T
  0.2254944037901560  0.0159983769250210  0.0567271081342097   T   T   T
  0.7552568531323627  0.0161832904830884  0.9030423711465453   T   T   T
  0.7552807793802669  0.0159215915081275  0.0568426975309429   T   T   T
  0.7255285193352418  0.5158742551355742  0.4027968148343726   T   T   T
  0.7255164343229467  0.5157832970952472  0.5565943956940782   T   T   T
  0.2552858224419696  0.5165354099009586  0.4027117913818178   T   T   T
  0.2552951231577367  0.5164687547948174  0.5565099710071552   T   T   T
  0.3227260540292316  0.1133038196872363  0.8061014080659468   T   T   T
  0.3998189836107063  0.1902032805704222  0.8828025545713820   T   T   T
  0.0874641913932080  0.3482112861087873  0.5706526374236188   T   T   T
  0.1648915560875559  0.4251395961488220  0.6469411000112053   T   T   T
  0.6253983484409535  0.0865489057669188  0.9800789357213633   T   T   T
  0.6643521814846224  0.9250776935264297  0.8123571632070811   T   T   T
  0.6580441262122879  0.1129919681989505  0.1543255158268590   T   T   T
  0.5816598782780898  0.1899138923256661  0.0769350747284616   T   T   T
  0.9902998921073327  0.5688299314416676  0.5791346544229151   T   T   T
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## Structure B

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## Structure F

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-0.1449430921386400 -0.0258498689395677 14.6380980218843586
Zr O C H
12 56 80 44
Selective dynamics
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