

Cite this: DOI: 10.1039/xxxxxxxxxx

## Supporting Information for: Square supramolecular assemblies of uranyl complexes in organic solvents<sup>†</sup>

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Received Date  
Accepted Date

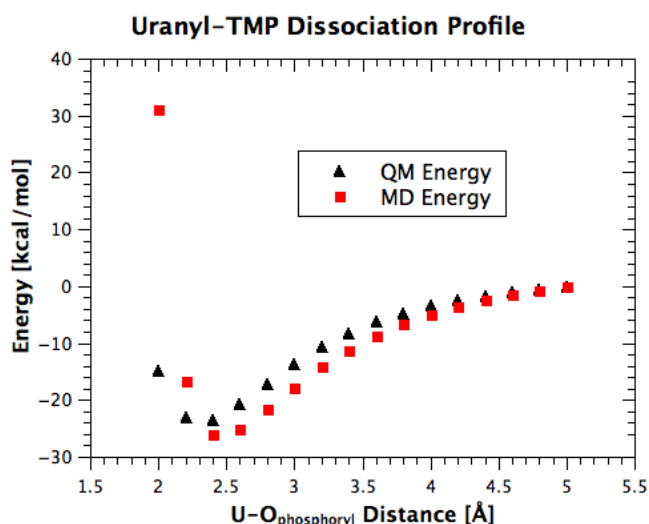
DOI: 10.1039/xxxxxxxxxx

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### 1 Simulation Methodology Background

Effective sampling of organic phase uranyl complexes in alkane solvents has substantial dynamic limitations. Quantification of the diffusion and association of those complexes requires accessing simulation times on the order of 100s of ns, which limits viable description of the interparticle interactions for molecular dynamics(MD) study to classical, nonpolarizable potentials. While existing nonpolarizable uranyl MD potentials are derived for aqueous solutions<sup>1–3</sup> where the uranium exhibits five-fold equatorial coordination, the organic phase  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_2$  complexes are six-coordinate<sup>4,5</sup>. Results from EXAFS<sup>4,5</sup> and UV-Vis<sup>5</sup> experiments show bidentate nitrate coordination of the uranyl, with the two coordinating TBP resulting in six-fold total coordination, for uranyl metal center for uranium and TBP concentrations ranging from nearly dilute to the solubility limit preceding third phase formation<sup>5</sup>. Therefore, while interactions between complexes increase with the concentration of those complexes, the well-characterized structure of the complexes themselves are unchanged. This contrasts with the monodentate nitrate  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_3$  and nitrate-bridging five-coordinate multi-uranyl complexes reported by Guilbaud *et al.* from MD simulations with polarizable potentials. We find that existing nonpolarizable uranyl potentials (which test a variety of charge assignments for the uranyl ion)<sup>1–3</sup> result in the formation of similar five-coordinate uranyl complexes. Therefore, the existing uranyl potentials are not applicable to modeling  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_2$  complexes. They underpredict ligand-uranium distances (forcing the five-fold coordination) and overpredict the corresponding interaction strength.

### 2 Force Field Parameterization



**Fig. 1** The QM and fitted MD dissociation energy profiles are plotted for TMP dissociation from the  $\text{UO}_2(\text{NO}_3)_2$  TMP complex.

Development of uranyl-ligand interaction potentials is necessary to accurately reproduce organic phase coordination and speciation of uranyl complexes. For this study, we parameterize a pair potential for the uranyl-extractant phosphoryl oxygen interaction by fitting a dissociation profile of TBP's lower homolog tri-methyl phosphate<sup>6</sup> from the uranium center of a  $\text{UO}_2(\text{NO}_3)_2(\text{TMP})_2$  complex. The uranyl-centered complex geometry was optimized using density functional theory (DFT) with the B3LYP functional and the Stuttgart ECP and basis set<sup>7</sup> for uranium and an aug-cc-pVDZ basis set for all other atoms. From that geometry, single point calculations were performed with 0.2 Å phosphoryl oxygen-uranium distance spacing from 2 to 5 Å using the same basis sets and second order Møller-Plesset perturbation theory. The uranium-phosphoryl oxygen Lennard-Jones (L-J) 12-6 potential was fitted with a least squares criterion on the

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<sup>†</sup> Electronic Supplementary Information (ESI) available. See DOI: 10.1039/b000000x/

difference in the gradient of the potential energy between MP2 and MD for rigid dissociation. The fitted TMP dissociation QM and MD energy profile is plotted in Figure 1. The fitted uranyl-phosphoryl oxygen sigma and epsilon parameters are 2.90016 Å and 0.19614 kcal/mol, respectively.

Uranyl and nitrate charges, which explicitly include charge transfer between the nitrate and uranyl, and the sigma and epsilon parameters for the remaining pairwise interactions are given in Table 1. The sigma and epsilon terms (along with harmonic bond and angle parameters) are taken from Kerisit and Liu<sup>3</sup> for uranyl and the Generalized AMBER Force Field (GAFF)<sup>8</sup> for nitrate. All L-J cross terms are derived from the standard Lorentz-Berthelot mixing rules. While the nitrate-uranium dissociation was similarly fit, the bidentate coordination of the nitrate in the  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_2$  complex was not stable in the presence of excess TBP in solution, forming  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_3$  structures with monodentate nitrates. To enforce the experimentally determined uranyl coordination environment, the nitrate nitrogen and coordinating oxygen positions were restrained to 0.299 to 0.301 nm and 0.249 to 0.251 nm, respectively, with a flat-bottom harmonic potential of 2390 kcal/(mol Å<sup>2</sup>). Interatomic distances from experiment<sup>4</sup>, DFT calculation and the resulting solution phase MD complex in *n*-dodecane, with restraints on nitrate-uranium distances and fitted uranyl-O<sub>TBP</sub> L-J pair potential, are given in Table 2. We have previously reported the force fields used for the extractant, organic solvent, water and nitric acid molecules<sup>9,10</sup>. Those previously implemented potentials include reparameterization of extractant and organic solvent potentials from the GAFF force field. The resulting force field was demonstrated to give excellent agreement with experiment for properties relevant to aggregation and solubility of the extractant, including dimerization constant<sup>11</sup>, volume change on mixing and enthalpy of mixing<sup>10</sup>. The NWChem software package<sup>12</sup> was used for all QM calculations and fitting was conducted using ForceFit<sup>13</sup>.

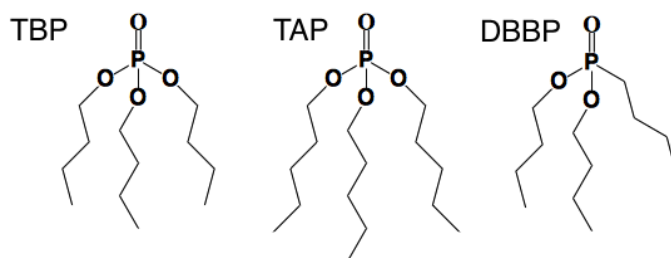
**Table 1** The charges, in units of elementary charge, are given for the uranyl nitrate complex along with the  $\sigma$  and  $\epsilon$  values for the uranyl and nitrate atoms.

| Atom                        | Charge [e] | $\sigma$ [Å] | $\epsilon$ [kcal/mol] |
|-----------------------------|------------|--------------|-----------------------|
| UO <sub>2</sub>             | 2.10       | 2.857        | 0.12                  |
| O <sub>UO<sub>2</sub></sub> | -0.45      | 3.125        | 0.20                  |
| N <sub>NO<sub>3</sub></sub> | 0.75       | 3.250        | 0.17                  |
| O <sub>NO<sub>3</sub></sub> | -0.45      | 3.000        | 0.17                  |

**Table 2** A comparison of interatomic distances for the  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_2$  complex between experiment<sup>4</sup> (solution phase), DFT optimization (this study, gas phase) and fitted MD (this study, solution phase, \* denoting restrained interatomic distances). The U-O<sub>NO<sub>3</sub></sub> oxygens are the bidentate coordinating oxygens of the nitrate and the U-O<sub>TBP</sub> oxygen is the phosphoryl oxygen of TBP.

| UO <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> (TBP) <sub>2</sub> atom pair | EXAFS <sup>4,5</sup> dist. [nm]               | DFT dist. [nm] | MD dist. [nm] |
|------------------------------------------------------------------------------|-----------------------------------------------|----------------|---------------|
| U-O <sub>NO<sub>3</sub></sub>                                                | 0.251 <sup>4</sup> , 0.247-0.250 <sup>5</sup> | 0.254          | 0.252*        |
| U-N <sub>NO<sub>3</sub></sub>                                                | 0.295-0.297 <sup>5</sup>                      | 0.299          | 0.298*        |
| U-O <sub>TBP</sub>                                                           | 0.241 <sup>4</sup> , 0.232-0.236 <sup>5</sup> | 0.243          | 0.240         |

### 3 MD Simulation Details



**Fig. 2** The molecular structure of the three extractants investigated in this study: TBP, TAP and DBBP.

Simulation compositions for each system are given in Table 3. Molecular structure of the three extractants in this study are shown in Figure 2. Compositions with excess TBP, and concomitant coextracted water and nitric acid, are taken from experimental data<sup>14</sup>. Initial configurations were generated using Packmol<sup>15</sup> with assembled  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_2$  complexes and solvent molecules randomly distributed within the simulation box. Simulations were conducted using the GROMACS 4.5.5 software package<sup>16</sup>. The isobaric isothermal NPT ensemble with periodic boundary conditions and leap-frog Verlet integrator was implemented with a 2 fs time step and the LINCS algorithm to constrain hydrogen-containing bonds. Pressure was set to 1 bar with the Parinello-Rahman barostat using a 2 ps time constant and temperature was set to 300 K with the Nosé-Hoover thermostat and a 0.2 ps time constant. A 1.5 nm cut-off was used for short range L-J and electrostatic interactions with Particle-Mesh Ewald summation for long range electrostatics. Production data for all systems was averaged over five trajectories of 60 ns, with the first 10 ns of each trajectory used for equilibration, yielding 250 ns of production time for each system.

### 4 Uranium-Uranium RDFs

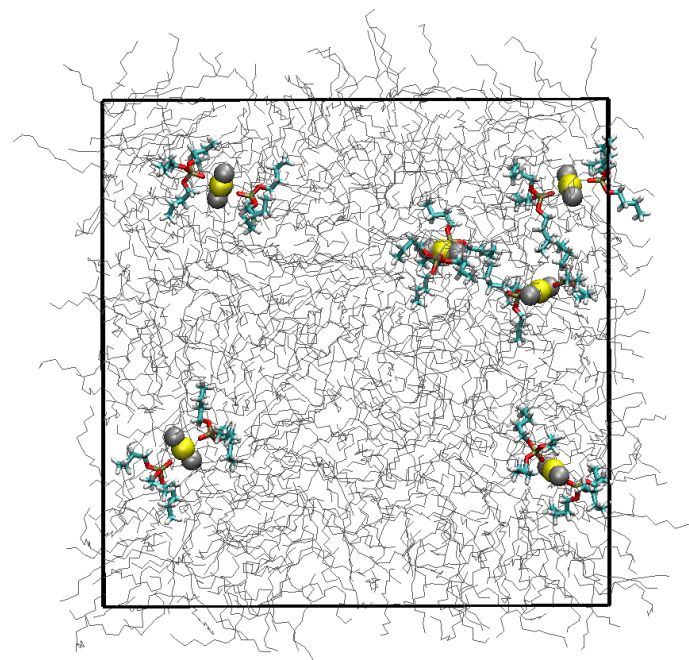
Figure 4 gives the uranium-uranium radial distribution functions (RDFs) for all simulation systems. The left panel shows that the primary correlation modes are consistent, although with different relative peak heights, between the low uranium concentration with pure *n*-dodecane solvent and the high uranium concentration with a process-like solvation environment. The middle panel shows that different extractants affect the relative peak heights while preserving the same correlation modes. DBBP significantly reduces the close-packed dimer while TAP has a reduced extractant-spaced dimer peak. The right panel shows the effects of different solvent conditions, including changing alkane chain length, “full” process solvation environment and a pure toluene solvent.

### 5 Comparison to Experimental X-ray Scattering

To demonstrate that the uranyl complexes and their solution phase self-association reported here are in agreement with experimental SAXS data, we compare that experimental scattering

**Table 3** Simulation system compositions and periodic cubic box lengths are given.

| System Label | Extractant Type | Solvent Type       | Number Extractant | Number Solvent | Number Uranyl Nitrate | Number Water | Number Nitric Acid | Cubic Box Dimension [nm] |
|--------------|-----------------|--------------------|-------------------|----------------|-----------------------|--------------|--------------------|--------------------------|
| I            | TBP             | <i>n</i> -dodecane | 12                | 604            | 6                     | 0            | 0                  | 6.18                     |
| II           | TBP             | <i>n</i> -dodecane | 131               | 604            | 40                    | 22           | 49                 | 6.68                     |
| III          | TBP             | <i>n</i> -hexane   | 298               | 1448           | 73                    | 43           | 0                  | 7.77                     |
| IV           | TAP             | <i>n</i> -dodecane | 12                | 604            | 6                     | 0            | 0                  | 6.19                     |
| V            | DBBP            | <i>n</i> -dodecane | 12                | 604            | 6                     | 0            | 0                  | 6.18                     |
| VI           | TBP             | <i>n</i> -hexane   | 12                | 1042           | 6                     | 0            | 0                  | 6.21                     |
| VII          | TBP             | <i>n</i> -dodecane | 131               | 604            | 6                     | 15           | 129                | 6.68                     |
| VIII         | TBP             | <i>n</i> -hexane   | 131               | 1042           | 6                     | 15           | 129                | 6.69                     |
| IX           | TBP             | toluene            | 12                | 1274           | 6                     | 0            | 0                  | 6.19                     |

**Fig. 3** A snapshot of the low uranium concentration simulation box is shown for the TBP/*n*-dodecane system.

profile reported by Guilbaud *et al.* to the simulation system with corresponding composition, system III, in Figure 5. The scattering intensity is calculated from the GROMACS gmx saxe tool with uranium Cromer-Mann coefficients added from Cromer and Mann<sup>17</sup>. Also plotted is the simulation profile also calculated by Guilbaud *et al.* from MD simulations using potentials with explicit polarizability and no restraints on atomic positions within the uranyl complex. Those simulations resulted in significant quantities of bridged uranyl species and monodentate nitrate, five-coordinate uranium  $\text{UO}_2(\text{NO}_3)_2(\text{TBP})_3$  complexes<sup>18</sup>. Figure 5 indicates that these differences in uranyl coordination do not result in substantial changes to the X-ray scattering profile: the correlation peak near  $14 \text{ nm}^{-1}$ , corresponding to a real space distance of  $0.45 \text{ nm}$  and characteristic of alkane and TBP/alkane solutions<sup>19,20</sup>, is present in both simulations. The scattering intensity at lower  $q$  values are in similar agreement with experiment. However, the scattering intensity from the simulation in this study is in much better agreement with experiment in the high  $q$  region. The deviation from experiment at high  $q$  in the literature simulation was present even for systems without uranium, indicating that the de-

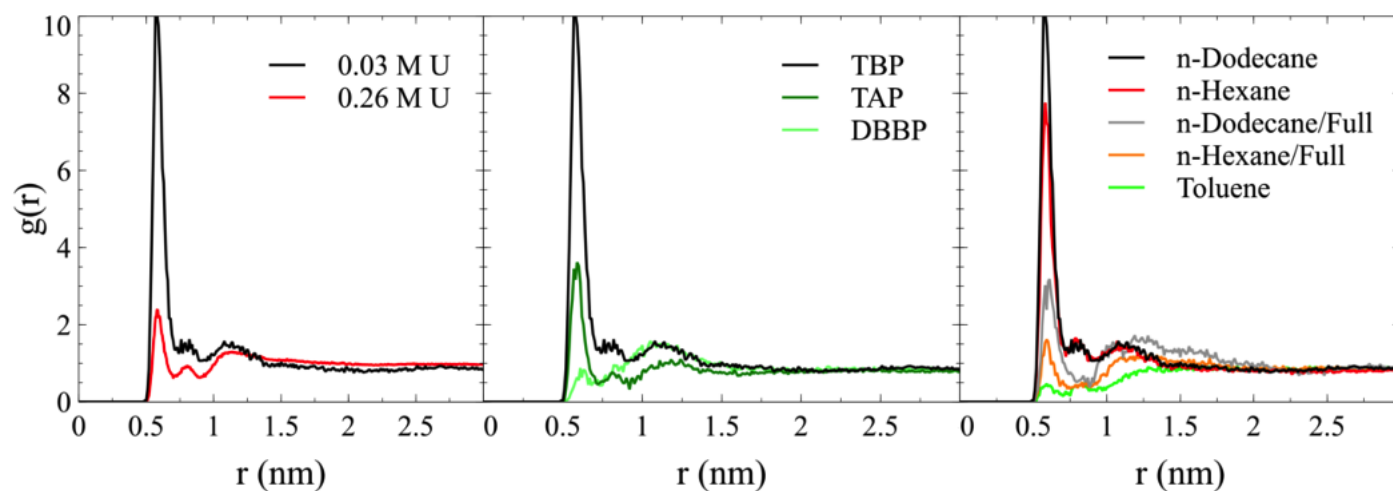
viation is unrelated to structural differences between the uranyl nitrate complexes but rather results from the TBP and alkane potentials implemented in that study. These data indicate that the X-ray scattering is largely insensitive to the differences between uranyl association for the nitrate bridged species and the associated uranyl complexes reported here. This could be a result of similar uranium-uranium distances for those two reported types of uranyl association. Therefore, we conclude that the simulations presented in this study, in addition to producing accurate uranyl coordination environment by construction, are not inconsistent with experimental X-ray scattering data.

## 6 Angles Between Extractants in Uranyl Dimer

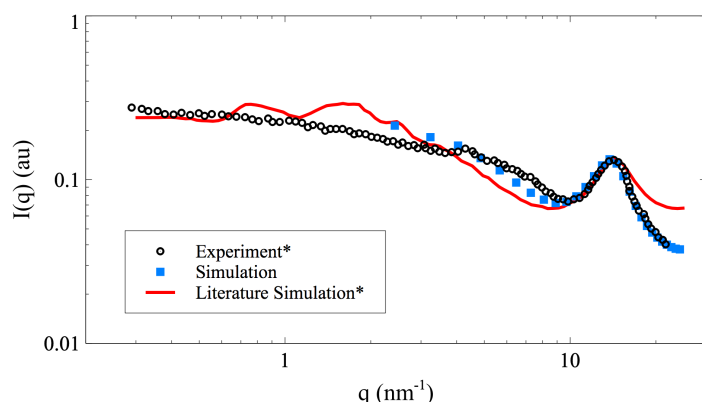
For the phosphorus-uranium-phosphorus angle distribution given in the main text, uranyl dimers were counted for uranium-uranium distances up to  $1.0 \text{ nm}$ . To compute the angle between extractants given by the phosphorus atom positions, if both TBP are in the same complex, the angle between the vectors from the uranium to the phosphorus atoms was calculated. If the TBP were in different uranyl complexes, one complex was chosen as a reference and the phosphorus atom positions of the other uranium complex were translated the vector connecting the uranium positions. Then, the angle between the phosphorus-uranium vector of the extractant coordinating the reference uranium and vector between the translated phosphorus and the reference uranium was computed. This process was conducted using reference uranium positions for both uranyl complexes in a dimer meaning that each dimer was counted twice, although the same phosphorus-uranium-phosphorus atom triplet angles are not necessarily exactly identical between both reference uraniums.

## 7 DFT and AIMD Methodology

Uranyl dimer configurations were taken from the classical MD trajectories with twenty-four explicit solvating *n*-hexane molecules. Those clusters were geometry optimized with Hatree-Fock (HF) theory for 50 steps with a 6-31G basis set for non-uranium atoms and the Stuttgart basis set and small ECP for uranium<sup>7</sup>. This was followed by 5 steps of HF optimization with a 6-31G\* for carbon and hydrogen and cc-pVDZ basis set for nitrogen, oxygen and phosphorus atoms. Lastly, the geometry was optimized for an additional 50 steps using DFT with the M05-2X functional and a 6-31G\* basis set for carbon and hydrogen, cc-pVDZ for oxygen, nitrogen and phosphorus and the Stuttgart basis set and small



**Fig. 4** The radial distribution functions are plotted for each system. The left panel compares the low concentration TBP/*n*-dodecane system compared to the uranium limiting organic concentration system for 20% TBP in *n*-dodecane with excess TBP and coextracted water and nitric acid representing process solvation conditions. The middle panel compares uranium correlation for the low uranyl concentration with TBP, TAP and DBBP. The right panel compares different solvents and solvation environments for TBP and the low uranium concentration.



**Fig. 5** The X-ray scattering intensity profiles from experimental data<sup>18</sup> (black circles) and literature simulation (red line) data<sup>18</sup> with the corresponding simulation system from this study (blue squares).

ECP for uranium. The M05-2X functional was chosen to adequately incorporate noncovalent interactions between the solvent molecules and uranyl nitrate/TBP complexes<sup>21–23</sup>. The series of optimization steps was chosen to assist SCF convergence. Further DFT optimization, while computationally expensive, is not expected to substantially change the structural character of the complexes as inter-complex geometries persisted during the optimization conducted. The final DFT geometry was used as the initial geometry for the AIMD simulation. The AIMD simulation was run in the NVT ensemble using the stochastic velocity rescaling thermostat to maintain a temperature of 300 K. A 20 a.u. time step was implemented for 216 total steps, corresponding to 104.5 fs trajectory length. All calculations were performed with the NWChem 6.8 software<sup>12</sup>.

## 8 DFT Geometries

In addition to the closely packed dimer structure discussed in the main text, three additional dimers were obtained from the

classical MD trajectory and subjected to the same DFT geometry optimization. All four DFT structures are shown in Figure 6 with dimer 1 discussed in the main text. Distances and angles, shown schematically in Figure 7, are provided in Tables 4 and 6 for all four closely packed dimer structures. For reference, the distances and angles from the initial MD clusters are given in Tables 5 and 7. For reference, the uranyl with its -yl oxygen interacting with the nitrogen center of a nitrate from the other uranyl is labeled as number 1. The other uranyl whose -yl oxygen interacts with the phosphorus atom of a TBP is labeled uranyl 2. These labels are shown in 7. As discussed in the main text, dimer 1 shows the square-shaped structural motif with the nitrate coordinating uranyl 2, interacting with the -yl oxygen of uranyl 1, rotated slightly out of the equatorial plane. In dimer 2, while also featuring the square structure, the entire uranyl 2 complex is rotated while the nitrate itself remains in the uranyl equatorial plane. This resulting largest change in the reported distances between this dimer and dimer 1 is the increased  $U_2-O_P$  distance. Dimer 3 is similar to dimer 1, although the uranyl complexes are spaced further apart with nearly all distances being larger than for dimer 1. In dimer 4, the -yl oxygen of uranyl 2 is positioned somewhat between the phosphate and nitrate of uranyl 1 instead of directly above the phosphate, while uranyl 2 nitrate is still rotated out of the equatorial plane as in dimer 1. While the square motif remains dominant for all of these dimers, there exist readily accessible variations in the distances and relative orientations of the uranyles and their ligands.

## 9 AIMD Simulation

Fluctuations in the dimer structure during AIMD simulation from the dimer 1 DFT geometry was measured to sample the local dimer configurational space at temperature. The distances reported in Table 4 are plotted over the length of the trajectory in Figures 8 and 9. Distances oscillated over the 100 fs trajectory with different, and multiple, periodicities. Most distances fluctu-

**Table 4** The distances are given for the four geometries from the DFT structures. Uranyl numbers correspond to labels given in Figure 7.

| Dimer Cluster | $O_N \dots U_2$<br>Dist. [Å] | $O_N \dots U_2$<br>Dist. [Å] | $O_{U_2} \dots P$<br>Dist. [Å] | $O_P \dots U_1$<br>Dist. [Å] | $O_{U_1} \dots N$<br>Dist. [Å] | $U_1 \dots U_2$<br>Dist. [Å] | $O_{U_1} \dots O_{U_2}$<br>Dist. [Å] | $O_{U_1} \dots U_2$<br>Dist. [Å] | $O_{U_2} \dots U_1$<br>Dist. [Å] |
|---------------|------------------------------|------------------------------|--------------------------------|------------------------------|--------------------------------|------------------------------|--------------------------------------|----------------------------------|----------------------------------|
| 1             | 2.536                        | 2.541                        | 3.026                          | 2.355                        | 2.893                          | 5.257                        | 3.112                                | 3.791                            | 4.149                            |
| 2             | 2.501                        | 2.529                        | 3.407                          | 2.390                        | 2.804                          | 5.201                        | 2.987                                | 3.927                            | 3.993                            |
| 3             | 2.520                        | 2.530                        | 3.411                          | 2.352                        | 3.115                          | 5.429                        | 3.323                                | 4.066                            | 4.241                            |
| 4             | 2.523                        | 2.556                        | 3.698                          | 2.381                        | 3.226                          | 5.178                        | 3.403                                | 4.003                            | 4.046                            |

**Table 5** The distances are given for the four geometries from the MD snapshots before DFT optimization. Uranyl numbers correspond to labels given in Figure 7.

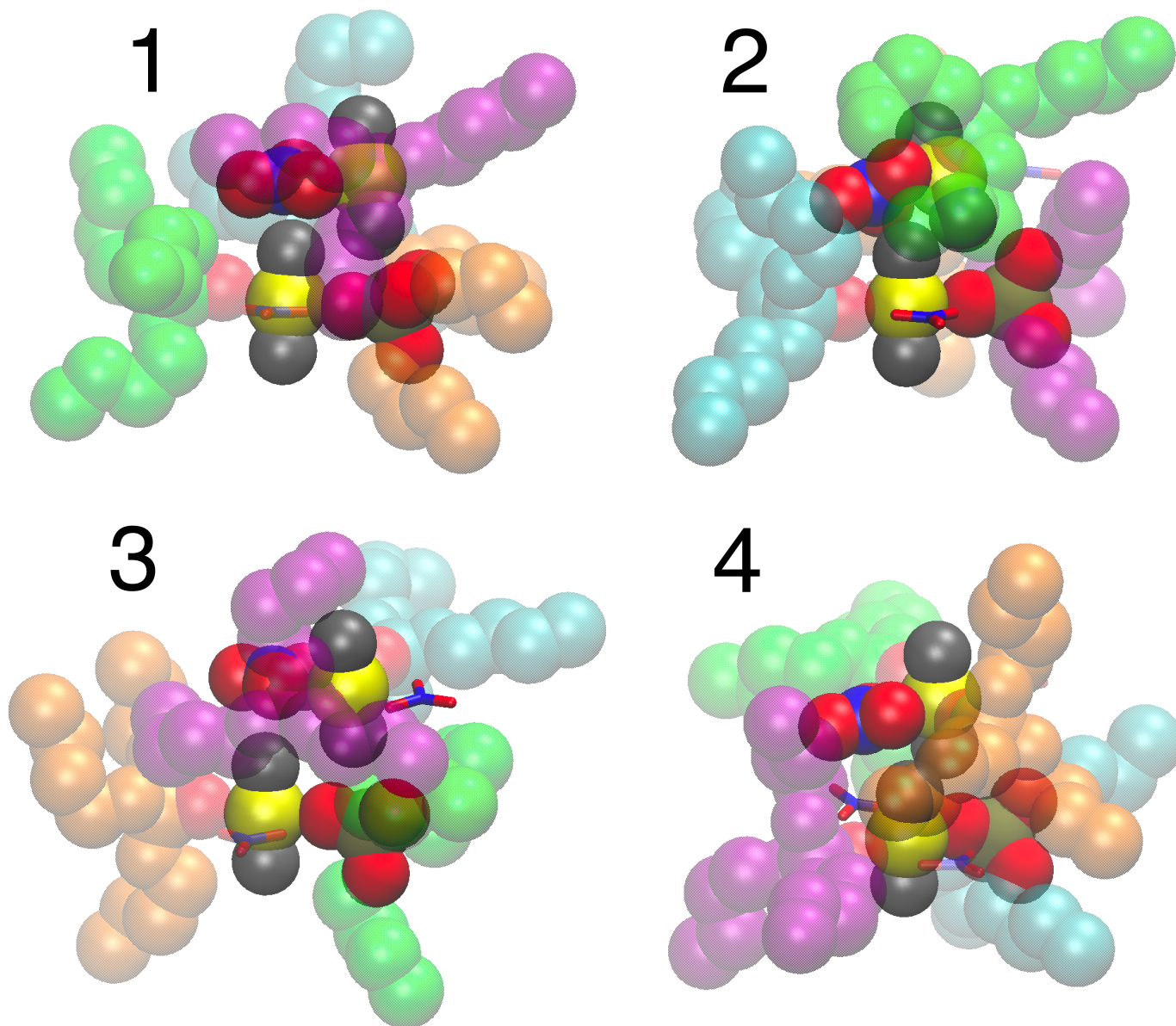
| Dimer Cluster | $O_N \dots U_2$<br>Dist. [Å] | $O_N \dots U_2$<br>Dist. [Å] | $O_{U_2} \dots P$<br>Dist. [Å] | $O_P \dots U_1$<br>Dist. [Å] | $O_{U_1} \dots N$<br>Dist. [Å] | $U_1 \dots U_2$<br>Dist. [Å] | $O_{U_1} \dots O_{U_2}$<br>Dist. [Å] | $O_{U_1} \dots U_2$<br>Dist. [Å] | $O_{U_2} \dots U_1$<br>Dist. [Å] |
|---------------|------------------------------|------------------------------|--------------------------------|------------------------------|--------------------------------|------------------------------|--------------------------------------|----------------------------------|----------------------------------|
| 1             | 2.554                        | 2.514                        | 3.273                          | 2.544                        | 3.192                          | 5.537                        | 3.340                                | 4.066                            | 4.381                            |
| 2             | 2.540                        | 2.512                        | 3.813                          | 2.398                        | 3.251                          | 5.478                        | 3.086                                | 4.222                            | 3.957                            |
| 3             | 2.489                        | 2.550                        | 3.674                          | 2.437                        | 2.779                          | 5.050                        | 2.898                                | 3.750                            | 3.674                            |
| 4             | 2.504                        | 2.523                        | 3.783                          | 2.368                        | 3.141                          | 5.203                        | 2.931                                | 3.776                            | 3.862                            |

**Table 6** The angles are given between the uranyl ions from the DFT structures. Uranyl numbers correspond to labels given in Figure 7.

| Dimer Cluster | $O_{U_1} = U_1 \dots U_2$<br>Ang. [deg.] | $O_{U_1} = U_1 \dots U_2$<br>Ang. [deg.] | $O_{U_2} = U_2 \dots U_1$<br>Ang. [deg.] | $O_{U_2} = U_2 \dots U_1$<br>Ang. [deg.] |
|---------------|------------------------------------------|------------------------------------------|------------------------------------------|------------------------------------------|
| 1             | 27.3                                     | 152.8                                    | 42.8                                     | 140.5                                    |
| 2             | 38.9                                     | 143.4                                    | 36.0                                     | 145.0                                    |
| 3             | 32.5                                     | 147.6                                    | 40.0                                     | 141.6                                    |
| 4             | 40.0                                     | 140.3                                    | 41.7                                     | 140.0                                    |

**Table 7** The angles are given between the uranyl ions from the MD snapshots before DFT optimization. Uranyl numbers correspond to labels given in Figure 7.

| Dimer Cluster | $O_{U_1} = U_1 \dots U_2$<br>Ang. [deg.] | $O_{U_1} = U_1 \dots U_2$<br>Ang. [deg.] | $O_{U_2} = U_2 \dots U_1$<br>Ang. [deg.] | $O_{U_2} = U_2 \dots U_1$<br>Ang. [deg.] |
|---------------|------------------------------------------|------------------------------------------|------------------------------------------|------------------------------------------|
| 1             | 29.2                                     | 148.4                                    | 43.4                                     | 139.7                                    |
| 2             | 39.4                                     | 143.1                                    | 28.9                                     | 153.5                                    |
| 3             | 36.0                                     | 150.1                                    | 33.1                                     | 150.2                                    |
| 4             | 30.9                                     | 146.9                                    | 35.1                                     | 145.9                                    |

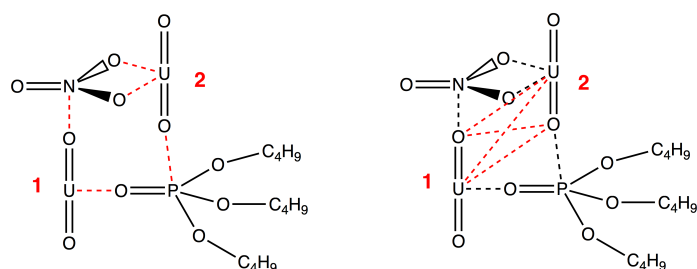


**Fig. 6** Snapshots are given of the four DFT dimers with no *n*-hexane shown for clarity.

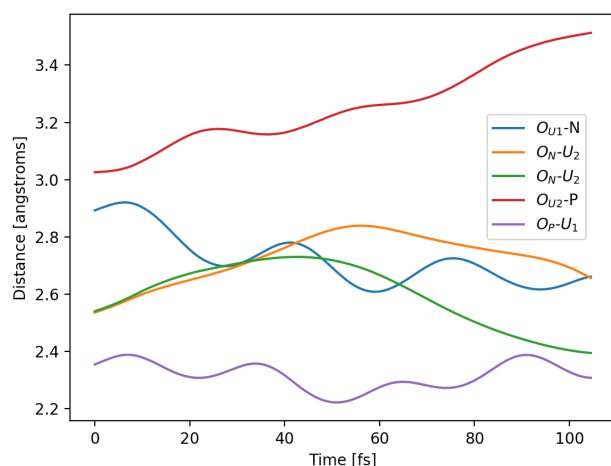
ated by up to 0.3 Å. While the  $OU_2$ -P distance increased for the entire trajectory, the predominant contribution to the increasing distance was the  $OU_2$  U=O double bond bending away from the phosphate group, and did not appear to correspond to a transition to another configuration. While the trajectory was not long enough to understand the dimer association dynamics observed in MD simulation which last up to 10s of ns, it indicates that detectable fs time scale fluctuations occur within the stable potential energy minimum of the square dimer structure.

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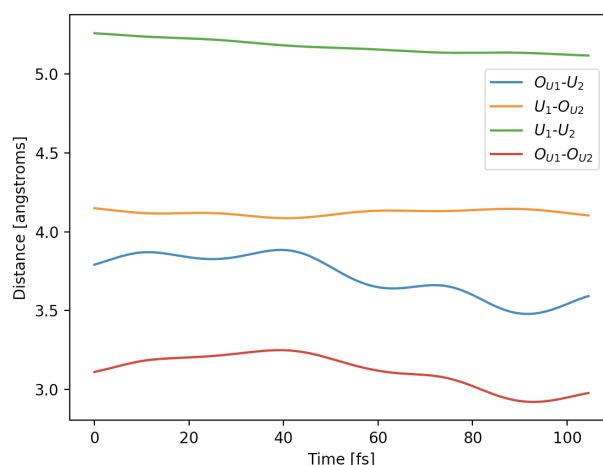
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**Fig. 7** The distances measured for the dimer configurations are shown here with the uranyles labeled as 1 and 2. The left schematic shows distances forming the square structural motif while the right shows distances measured between the uranyl ions themselves.



**Fig. 8** Fluctuations in inter-complex distances of dimer 1 during the AIMD trajectory starting from the DFT geometry are plotted with uranyl labels given in Figure 7.



**Fig. 9** Fluctuations in distances between the uranyl cations of dimer 1 during the AIMD trajectory starting from the DFT geometry are plotted with uranyl labels given in Figure 7.

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## 10 Appendix A: Dimer .xyz coordinates

### 10.1 Cluster 1

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