

Enhancing DFT-based energy landscape exploration by coupling Quantum Mechanics and Static Modes

Supplementary Information

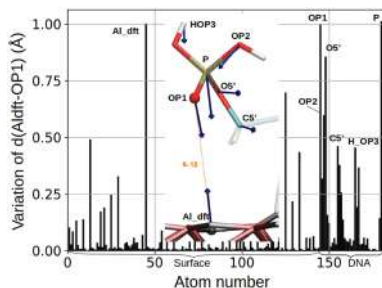
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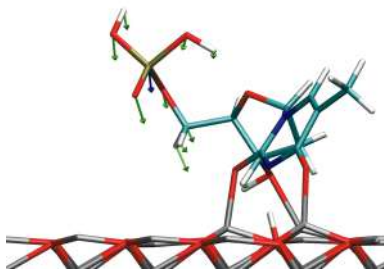
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S1. Supplementary Material 1

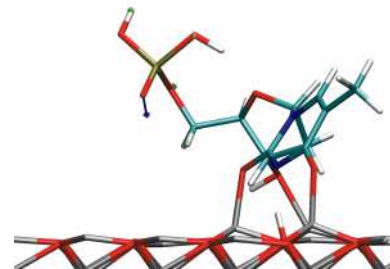
(a) Variations of the distance $d(\text{OP1-Al-dft})$ induced by the optimized excitation of each atom of the Configuration Up. (b) System deformation field with associated directions of the forces applied on the P atom from Up configuration. (c) System deformation field with associated directions of the forces applied on the OP1 atom from Up configuration. (d) System deformation field with associated directions of the forces applied on the O5' atom from Up configuration. (e) System deformation field with associated directions of the forces applied on the OP2 atom from Up configuration. (f) System deformation field with associated directions of the forces applied on the C5' atom from Up configuration.



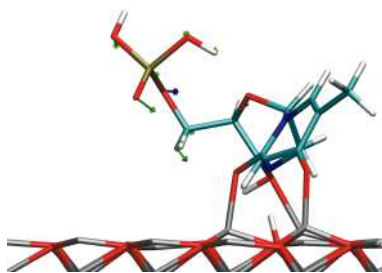
(a) Optimized stress



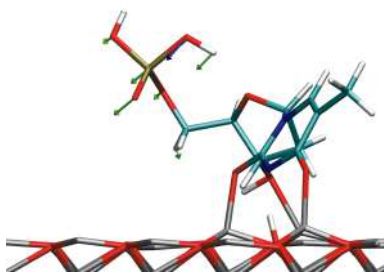
(b) Deformation field by P



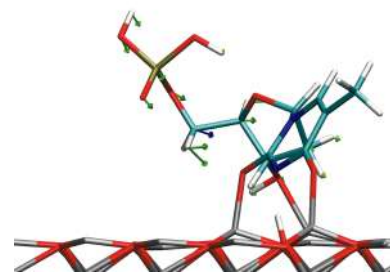
(c) Deformation field by OP1



(d) Deformation field by O5'



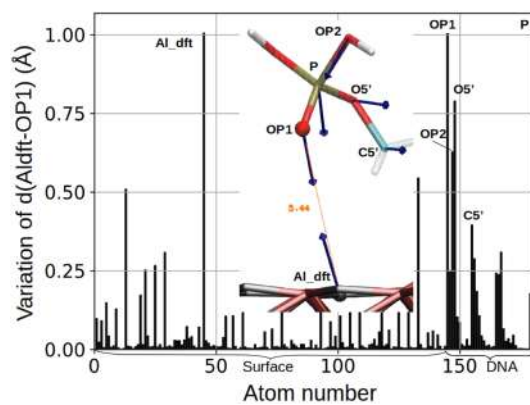
(e) Deformation field by OP2



(f) Deformation field by C5'

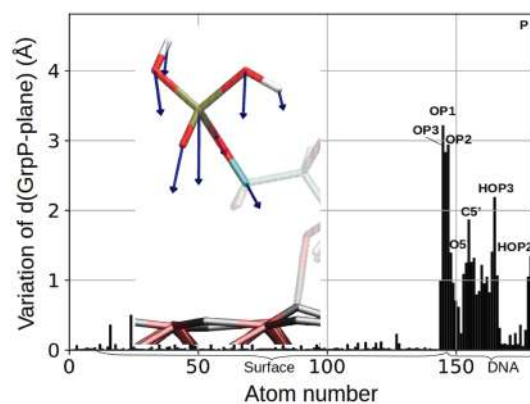
S2. Supplementary Material 2

Histogram to compare atom influence on the variation of distance $d(\text{OP1-Al-dft})$ from configuration B.



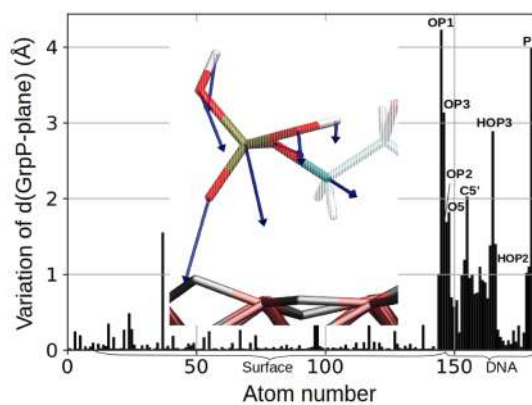
S3. Supplementary Material 3

Histogram to compare atom influence on the variation of the sum of distance between the phosphate group atoms and the surface from configuration A (Up).



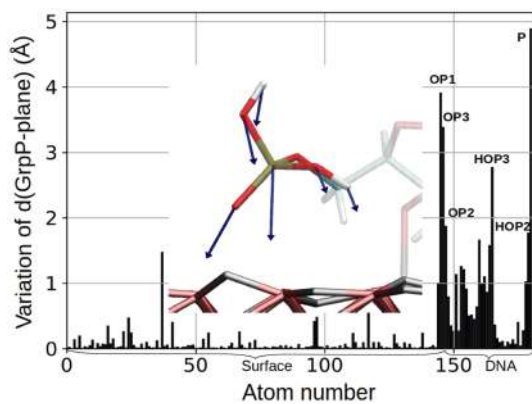
S4. Supplementary Material 4

Histogram to compare atom influence on the variation of the sum of distance between the phosphate group atoms and the surface from configuration E.



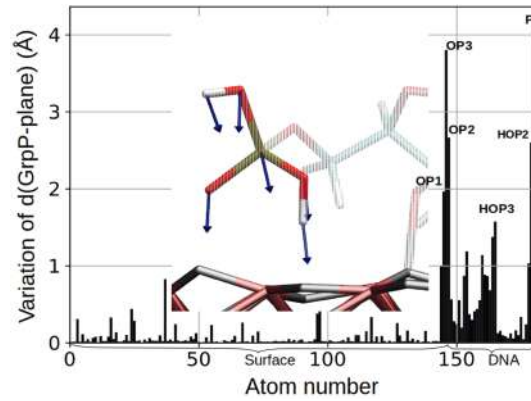
S5. Supplementary Material 5

Histogram to compare atom influence on the variation of the sum of distance between the phosphate group atoms and the surface from configuration F.



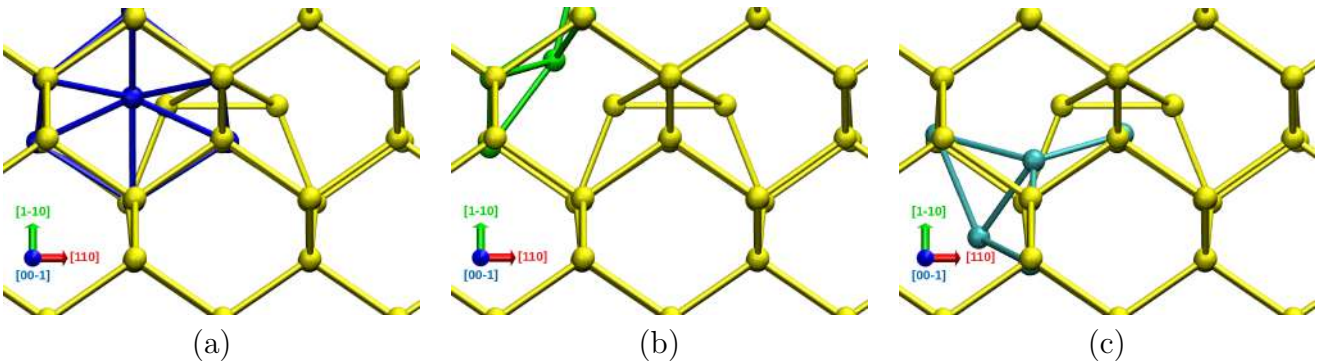
S6. Supplementary Material 6

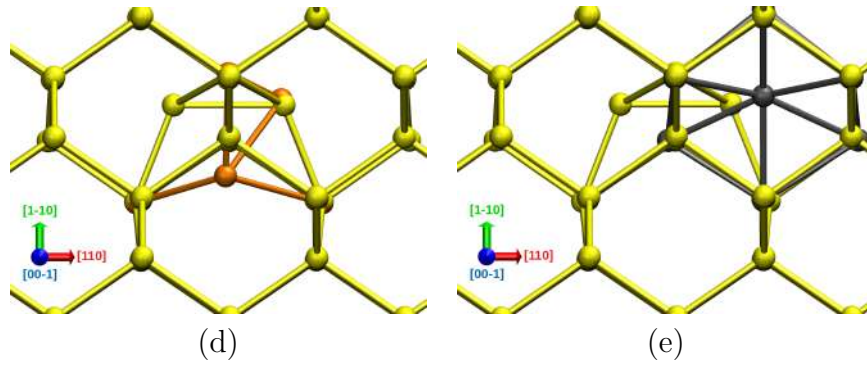
Histogram to compare atom influence on the variation of the sum of distance between the phosphate group atoms and the surface from configuration G.



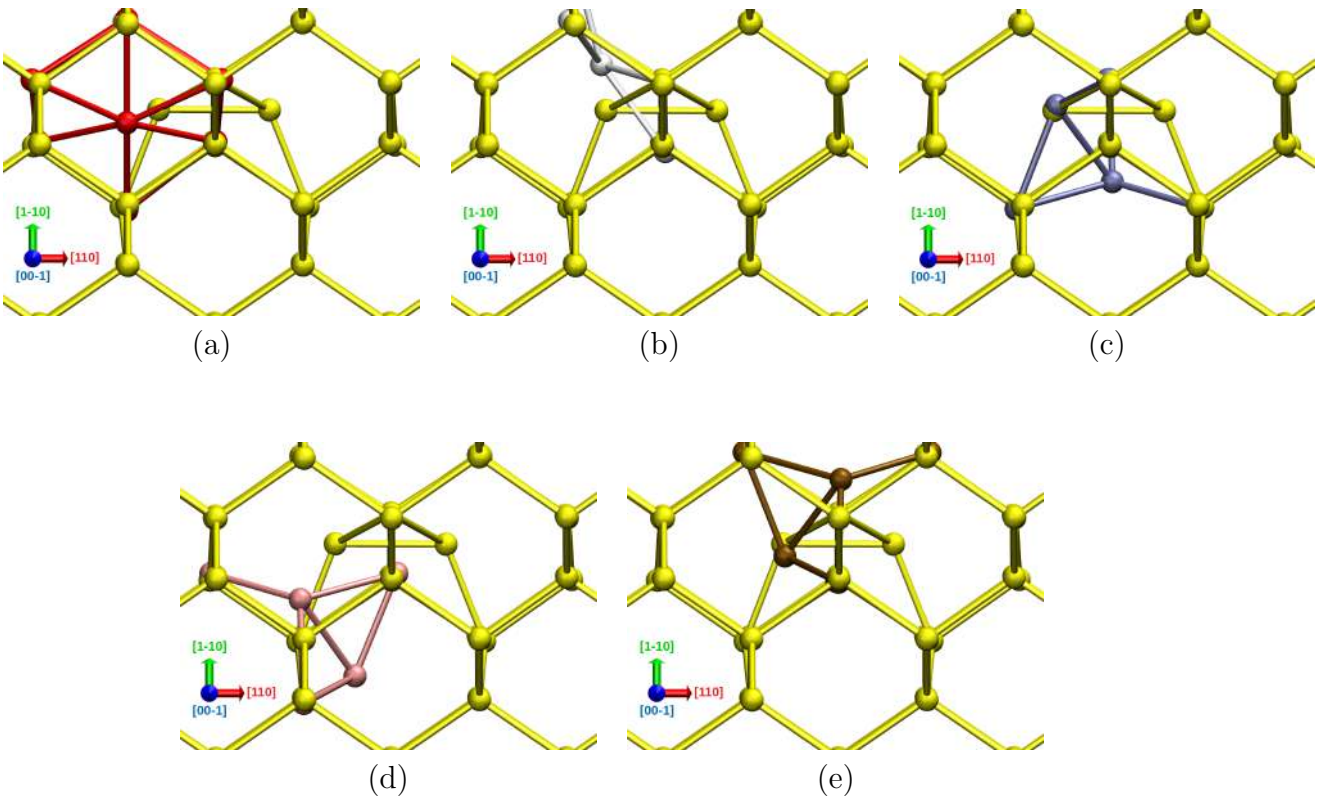
S7. Supplementary Material 7

Configurations reached by QMSM from Si Dumbbell configuration (called yellow), as presented in Figure 7(b) and Table 2 in the article. (a) H blue. (b) H green. (c) D cyan. (d) D orange. (e) H black.





Configurations reached by QMSM from Si Hexagonal configuration (called blue), as presented in Figure 8(b) and Table 3 in the article. (a) H red. (b) H white. (c) D purple. (d) D pink. (e) H brown.



S8. Supplementary Material 8

Intermediate configurations encountered in I_4 migration. (a) Configuration TIS-1'. (b) TIS-2' configuration. (c) TIS-2'' configuration.

