Tutorial For QUBEMAKER

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In order to create a QUBE force field three stages are required. The protein structure is first minimized using OPLS-AA/M (and a '.psf' file created), the ONETEP calculation is then carried out and the '.psf' file and '.onetep' file is then used to create the QUBE files.

1 ONETEP Input Structure

We suggest that the input structure used for the ONETEP calculation is the experimental protein structure minimized with OPLS-AA/M in a water box. Instructions on how to create NAMD input files using VMD are given here:
https://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-unix-html/.
The required topology files for OPLS-AA/M are supplied at:
http://zarbi.chem.yale.edu/oplsaam.html.[1]
A .psf file created with the OPLS-AA/M topology file is required to build the QUBE force field as the OPLS atom types dictate the bonded parameters assigned.

With the require '.psf' and '.par' OPLS-AA/M files, the protein can be minimized using NAMD. The minimized protein structure can then be converted to a '.xyz' file format and used for the ONETEP calculation.

2 ONETEP Calculation

The ONETEP calculation used to create the QUBE force field is now outlined. Four nonorthogonal generalised Wannier functions (NGWFs) were used for all atoms with the exception of hydrogen which used one. The NGWFs had a radii of 10 Bohr. The periodic sine (psinc) basis was used to describe the NGWFs, with a grid size employed that corresponds to a plane wave cutoff energy of 1020 eV. The PBE exchange-correlation functional

was used with PBE OPIUM norm-conserving pseudopotentials.[2] Partitioning of the polarized ground-state electron density was performed using the DDEC scheme in ONETEP with the mixing parameter (γ) set to 0.02.

The ONETEP calculation will output a '.onetep' file. This '.onetep' file is required to create the QUBE force field files.

3 Using QUBEMAKER

Two files are required to build a new QUBE force field. A 'ddec.onetep' files from the ONETEP calculation, and a 'ionized.psf' file creating with the VMD software and the OPLS-AA/M topology file. In order to run the program, a new folder in the 'Input_File' should be created to contain the input files. The variable 'folder_name' at the top of the 'full_force_field_creation.m' script should then be changed to the name of this new folder. Running the 'full_force_field_creation.m' script will create the new QUBE force field by using the information from the two input files. This will take a couple of minutes and will result in new files created in the folder 'Final_File'. Two new files are present in a subdirectory of this folder, a 'QUBE_FF.inp' and 'new_ionized.psf' file. These two new files can then be used with the NAMD program.

References

(1) Robertson, M. J.; Tirado-Rives, J.; Jorgensen, W. L. Improved Peptide and Protein Torsional Energetics with the OPLS-AA Force Field. *J. Chem. Theory Comput.* **2015**, *11*.

(2) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made sim-

ple. *Phys. Rev. Lett.* **1996**, *77*.