The head disk interface in hard disk drive can be considered one of the hierarchical multiscale systems, which require the hybridization of multiscale modeling methods with coarse-graining procedure. However, the fundamental force field parameters are required to enable the coarse-graining procedure from atomistic/molecular scale to mesoscale models .In this paper, we investigate beyond molecular level and perform *ab-initio* calculations to obtain the force field parameters. Intramolecular force field parameters for the Zdol and Ztetraol were evaluated with truncated PFPE molecules to allow for feasible quantum calculations while still maintaining the characteristic chemical structure of the end groups. Using the harmonic approximation to the bond and angle potentials, the parameters were derived from the Hessian matrix, and the dihedral force constants are fit to the torsional energy profiles generated by a series of constrained molecular geometry optimization.