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Force Field Parameterization and Property Calculation of Aminofluorene-Based Chromophores DAVID RIGBY, Accelrys, Inc, RAJIV BERRY, AFRL/MLBP, Wright Patterson AFB — In recent years, a variety of aminofluorene-based chromophores have been synthesized and studied experimentally for potential use in applications ranging from high density storage and imaging to detection of chemical and biological agents. In view of the large number of compounds of this type, it is desirable to be able to perform property prediction on interesting molecules as efficiently and accurately as possible – a need which may be realized by use of molecular modeling techniques in combination with increasingly accurate force fields. Currently the most significant obstacle to accurate property prediction is the lack of accurate force field parameters for the chromophore functional groups of interest. Accordingly, we have performed ab-initio based valence parameter development combined with a classical approach to nonbond parameter refinement (as employed for the COMPASS force field) for relevant model compounds. The resulting force field has then been applied to investigate prediction of properties, including glass transition temperatures, for several molecules of interest.

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