

Publication

A Supervised Fitting Approach to Force Field Parametrization with Application to the SIBFA Polarizable Force Field

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)**ID** 2834792**Author(s)** Devereux, Mike; Gresh, Nohad; Piquemal, Jean-Philip; Meuwly, Markus**Author(s) at UniBasel** [Meuwly, Markus](#) ; [Devereux, Michael](#) ;**Year** 2014**Title** A Supervised Fitting Approach to Force Field Parametrization with Application to the SIBFA Polarizable Force Field**Journal** Journal of Computational Chemistry**Volume** 35**Number** 21**Pages / Article-Number** 1577-91**Keywords** SIBFA, polarizable force field, parametrization, parameter fitting, I-NoLLS**Mesh terms** Computer Simulation; Formamides, chemistry; Imidazoles, chemistry; Magnesium, chemistry; Models, Chemical; Water, chemistry

A supervised, semiautomated approach to force field parameter fitting is described and applied to the SIBFA polarizable force field. The I-NoLLS interactive, nonlinear least squares fitting program is used as an engine for parameter refinement while keeping parameter values within a physical range. Interactive fitting is shown to avoid many of the stability problems that frequently afflict highly correlated, nonlinear fitting problems occurring in force field parametrizations. The method is used to obtain parameters for the H₂O, formamide, and imidazole molecular fragments and their complexes with the Mg²⁺ cation. Reference data obtained from ab initio calculations using an aug-cc-pVTZ basis set exploit advances in modern computer hardware to provide a more accurate parametrization of SIBFA than has previously been available. (C) 2014 Wiley Periodicals, Inc.

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