Computational Chemical Dynamics: From Gas–Phase to Condensed–Phase Systems

Poster Presentations

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6:30–10:00 p.m.

Great Hall
Coffman Memorial Union
University of Minnesota
Minneapolis, Minnesota
Poster A13

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CP2K-MC: A Monte Carlo Approach for First Principles Simulations

A simulation method for performing Monte Carlo simulations from first principles is presented. The Monte Carlo code is written using the energy routines from CP2K, which evaluates energies using an atom-centered primary basis set and a plane-wave auxiliary basis set. Calculations were performed using density functional theory, using the BLYP exchange/correlation functionals. Simulations on water were run in the canonical, isobaric-isothermal, and Gibbs ensembles. Final results for the canonical ensemble are shown, along with preliminary results in the isobaric-isothermal and Gibbs ensembles. The results are compared to classical simulations and experimental results.

Poster A14(i)

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Estimation of Tissue:Air Partition Coefficients: A Comparison Of Structure- and Property-Based Methods

Tissue:air partition coefficients are important in understanding the toxicokinetics of chemicals and in developing physiologically-based pharmacokinetic (PBPK) models. Three linear regression methods were used to develop models for the prediction of tissue:air partition coefficients including fat:air, liver:air and muscle:air for male Fischer 344 rats. The models were developed with a set of 46 diverse low molecular weight volatile compounds, as well as a subset of 26 haloalkanes. Comparisons were made between models utilizing strictly structure-based descriptors and property-based descriptors including saline:air and olive oil:air partition coefficients. The results indicated that ridge regression (RR) generally outperformed principal component regression (PCR) or partial least squares (PLS) regression. The models involving structure-based descriptors were comparable to, and in some cases superior to, models utilizing property-based descriptors. Some descriptor types, including molecular weight, low-order valence connectivity indices and descriptors of cycllicity and aromaticity, were found to be important for the prediction of all three partition coefficients; while descriptors representing polarity and hydrogen bonding were important only for the prediction of liver:air and muscle:air partition coefficients.

Poster A14(ii)

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Use of Topological Indices in Predicting Aryl Hydrocarbon (Ah) Receptor Binding Affinity of Dibenzofurans: A Hierarchical QSAR Approach

Dibenzofurans are widespread environmental contaminants that are produced mainly as undesirable by-products in natural and industrial processes. The toxic effects of these compounds are thought to be mediated through binding to the aryl hydrocarbon (Ah) receptor. In this study, we have used our HiQSAR approach in the development of QSAR models to predict Ah receptor binding affinity utilizing a set of 34 dibenzofurans. Topostructural (TS), topochemical (TC), geometrical (3D), and ab initio (sto-3g) quantum chemical indices have
been employed either alone or hierarchically in the development of the QSAR models. Results show that, for the full set, the TS and TC indices explain most of the variance in the data. The addition of 3D and quantum chemical indices results in only slight improvement in the predictive capability of QSAR models.

**Poster A15**

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*Hierarchical Quantitative Structure-Activity Relationship (HiQSAR) Studies of Mosquito Repellency of Alicyclic Carboxamides*

In the quest for finding alternatives for the most popular topical repellant, N,N- Diethyl-3-methylbenzamide (DEET), development of QSAR models play a very important role because these models can be used to tailor the similarity space and select compounds from large data sets in the identification of leads. Mosquito repellency data of alicyclic carboxamides for *Aedes aegypti* and *Anopheles quadrimaculatus* are modeled by Hierarchical Quantitative Structure-Activity Relationship (HiQSAR) technique using topostructural, topochemical, geometrical, and quantum mechanical parameters. Three types of multiple regression methods namely, ridge regression, regression using principle components extracted from the independent variables, and partial least square analysis were applied. In all the three methods Topostructural parameters are found to correlate well with the time of protection and there was no improvement in the model on adding topochemical, geometrical and quantum chemical parameters. This indicates that structural factors like size and shape of the repellent is the primary factor that governs the repellency of the carboxamides.

**Poster A16**

Kim Palmo and Samuel Krimm
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*SDFF Potential Energy Functions: Theoretical Basis and Accuracy of a Non-Iterative Polarization Model*

Our spectroscopically determined force field (SDFF) methodology [1] is briefly reviewed, with emphasis on the importance of constructing physically accurate energy functions. SDFF extensions and philosophical differences with respect to standard empirical force fields are elaborated.

As part of our efforts to include many-body interactions into the force field, we have analyzed the theory of dipole polarization and derived the difference in induction energy between an iterative (self-consistent) and non-iterative (one-step) scheme [2]. We conclude that this difference is bound to be small in most cases, so that a non-iterative polarization model can be expected to give a satisfactory representation of the induction energy. This is demonstrated with examples of configurations of water molecules. Advantages of a one-step procedure are discussed.